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# The Coulomb Green functions with applications to two photon transitions.

Robin Andrew Swainson  
*University of Windsor*

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THE COULOMB GREEN FUNCTIONS  
with applications to two photon transitions.

by  
Robin Andrew Swainson

Submitted to the  
Faculty of Graduate Studies and Research  
through the Department of Physics  
in partial fulfillment of the requirements for  
the Degree of Doctor of Philosophy  
at the University of Windsor

Windsor, Ontario, Canada

- 1988

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DEDICATED

with love and gratitude to my parents

Gwen and Denis Swainson

and

to the memory of my friend and colleague

Dr. Paul D. Kirkman (1959–1986).

## ABSTRACT

A comprehensive examination of the properties of the Schrodinger- and Dirac-Coulomb Green function as applied to bound state problems is presented. A method of treating the Dirac-Coulomb radial equations is described which allows both the Dirac wavefunctions and Green functions to be treated quite analogously to the corresponding Schrodinger functions. Matrix elements in the form of double Laplace transforms of the Green functions are calculated and presented in a variety of useful forms. The results are applied specifically to two photon transitions in hydrogenic ions, with a calculation of the decay of the  $2s_{1/2}$  state.

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## TABLE OF CONTENTS

ABSTRACT.....	iv
ACKNOWLEDGEMENTS.....	v
LIST OF TABLES.....	viii
CHAPTER 1: INTRODUCTION.....	1
CHAPTER 2: THE SCHRODINGER- AND DIRAC-COULOMB EQUATIONS	
2.0: Introduction.....	10
2.1: The Schrodinger-Coulomb Equation.....	11
2.2: The Dirac-Coulomb Equation.....	21
2.3: Recursion relations and other properties of the Coulomb radial wavefunctions.....	32
CHAPTER 3: THE SCHRODINGER-COULOMB GREEN FUNCTION	
3.0: Reduction to the radial equation.....	39
3.1: Solution of the generalized radial equation.....	40
3.2: Forms of the Schrodinger-Coulomb Green function.....	45
3.3: An integral equation.....	52
CHAPTER 4: THE DIRAC-COULOMB GREEN FUNCTION	
4.1: Reduction to the radial equation.....	53
4.2: Transformation of the radial equations.....	55
4.3: Forms of the radial Dirac-Coulomb Green function.....	59
4.4: Reduction to the nonrelativistic limit.....	63

## CHAPTER 5: THE DOUBLE LAPLACE TRANSFORMS OF THE COULOMB GREEN FUNCTIONS

5.0: Introduction.....	65
5.1: DLT's of the Schrodinger-Coulomb Green function.....	65
5.2: DLT's of the Dirac-Coulomb Green function.....	74
5.3: A generalized DLT of the radial Coulomb Green functions.....	77
5.4: Inverting the variables in the DLT of $g_{\ell}$ .....	82

## CHAPTER 6: THE REDUCED COULOMB GREEN FUNCTIONS

6.1: The reduced Schrodinger-Coulomb Green function.....	85
6.2: The DLT of the reduced Schrodinger-Coulomb Green function.....	90

## CHAPTER 7: TWO PHOTON BOUND STATE- BOUND

### STATE TRANSITIONS IN ATOMIC HYDROGEN

7.1: Introduction.....	92
7.2: The Theory of Two photon transitions.....	93
7.3: The nonrelativistic two photon decay of the $2s_{1/2}$ level of hydrogenic ions.....	102

## APPENDICES

A.1: Special functions.....	112
B.1: Calculation of some integrals required for the normalization of wavefunctions.....	114
B.2: A simplified form of $F_1$ when two parameters are integers.....	116
B.3: The Laplace transform of the spherical Bessel function.....	118
B.4: On the function ${}_2F_1(M+N+1,1;N+1;X)$ .....	122
B.5: On a sum related to the logarithm.....	123
REFERENCES.....	124
VITA AUCTORIS.....	127

## LIST OF TABLES

1. Spectral Distribution in the Long wavelength approximation.....110
2. Spectral Distribution for  $Z=1$  &  $Z=20$ .....111

## CHAPTER 1 : INTRODUCTION

An analysis of the spectroscopy of the hydrogen atom eventually necessitates consideration of processes involving two photons. In the first approximation the lifetime of a hydrogenic state depends upon the degree to which it is able to make transitions to lower lying states with the emission of a single photon. Often a state will be stable to simple electric dipole transitions as a consequence of a selection rule. Then higher multipole transitions must be considered. It may be that relativistic corrections to the transition rates must also be taken into consideration, as well as corrections to the so-called long wavelength approximation. And finally, it often happens that a state stable to single photon decay can decay to lower lying states with the simultaneous emission of two or more photons. Thus any theoretical calculation of the lifetime of the state will require knowledge of the two-photon transition rates.

The basic mathematical analysis required to attain such knowledge can be equally well applied to other processes involving two photons. We have just described two-photon bound state transitions. Virtually the same analysis will allow us to consider two photon ionization, or bound-free transitions. The absorption of a single photon followed by its immediate re-emission, that is the scattering of photons by the hydrogen atom which is itself left either in an excited or a fully ionized state is also subsumed in the analysis. Even the bound electron self energy, the Lamb shift, which is a process involving the emission and subsequent re-absorption of a single virtual photon requires basically the same mathematical formalism for its solution.

Naturally several techniques have been used to examine these processes. Common to all of them is the necessity to treat the Coulomb Green function in some appropriate manner. One can attempt to bypass the Green function by solving an inhomogeneous differential equation, the so-called Dalgarno-Lewis perturbation method.<sup>1,2</sup> This has been used successfully since the 1950's. Then again one may attempt to represent the Green function by a finite set of variationally determined wavefunctions, a technique which has been used with increasing success over the past decade or so.<sup>3</sup> Finally one may hope to use exact analytical forms of the Green function and from those derive the matrix elements required.<sup>4,5</sup> This last approach provides the motivation for the work presented here.

In the following chapters I attempt to present a self-contained and consistent treatment of both the nonrelativistic and relativistic Green functions for hydrogenic ions. The relativistic case is presented in a manner which closely resembles the non-relativistic case; this then allows for the computation of matrix elements in an equally similar manner. These matrix elements, which are effectively double Laplace transforms of the radial part of the Green functions are given in several different forms, with as few restrictions on the range of parameters as possible. Thus I avoid the necessity of introducing the parametric differential operators which frequently appear in such calculations.<sup>5</sup> The analysis is then applied to a particular physical calculation, that of the nonrelativistic two-photon decay of the 2s level of atomic hydrogen with retardation.

At this point it is convenient to examine briefly just what is meant by the Green function of an operator. Given a Hermitian operator  $H$  the corresponding resolvent or Green operator  $G(z)$  is defined by

$$(H - z) G(z) = 1 \quad (1.1)$$

where  $z$ , referred to later on as the 'energy variable' is a complex number. Usually  $H$  will have associated with it a complete set of eigenfunctions  $\psi_E$  corresponding to generally both discrete and continuous eigenvalues  $E$ , so that

$$(H - E) \psi_E = 0, \quad (1.2)$$

$$\sum \psi_E \psi_E^\dagger = 1. \quad (1.3)$$

It is now obvious that a formal expression for  $G(z)$  is given by

$$G(z) = \sum \psi_E \psi_E^\dagger / (E - z). \quad (1.4)$$

If  $H$  is represented by a differential operator  $H_r$  acting on a Hilbert space of functions on  $\mathbb{R}^3$ ,  $G(z)$  is itself represented by a function  $G(\mathbf{r}_1, \mathbf{r}_2; z)$  on  $\mathbb{R}^3 \times \mathbb{R}^3$  which satisfies

$$(H_{r_1} - z) G(\mathbf{r}_1, \mathbf{r}_2; z) = \delta(\mathbf{r}_1 - \mathbf{r}_2). \quad (1.5)$$

We shall be concerned here exclusively with the Schrodinger- and Dirac-Coulomb Green functions. In view of the nature of the Hamiltonians involved we see that the former will be a scalar function, while the latter will be a  $4 \times 4$  matrix-valued function.

The Schrodinger-Coulomb Green function  $G(\mathbf{r}_1, \mathbf{r}_2; z)$  is defined to be the solution (with appropriate boundary conditions) of<sup>6</sup>

$$\left[ -\frac{\hbar^2}{2m} \nabla_1^2 - \frac{\hbar^2}{amr_1} - z \right] G(\mathbf{r}_1, \mathbf{r}_2; z) = \delta(\mathbf{r}_1 - \mathbf{r}_2). \quad (1.6)$$

Here  $m$  is the electron mass,  $a = a_0/Z$  is the scaled Bohr radius for a nucleus with charge  $Z$ , and  $\hbar$  is Planck's constant. In view of the hermitian nature of the Hamiltonian we see that  $G(\mathbf{r}_1, \mathbf{r}_2; z) = G^\dagger(\mathbf{r}_2, \mathbf{r}_1; z)$ . There have been a number of methods used to determine the functional form of  $G$ , ranging from the direct computation of the sum in (1.4), to expansions as sums of products of radial functions and angular functions, solution in parabolic coordinates, solution in momentum space, and solutions in phase space.

It appears that the first published attempt to calculate the Schrodinger-Coulomb Green function was by Meixner<sup>7</sup> in 1933 where he only partially succeeded in solving the three-dimensional problem in parabolic coordinates. Following that, a solution of the radial functions was discovered involving the product of an homogeneous Whittaker function with an inhomogeneous one. Integral representations for the full Green function in coordinate space were not found until the 1960's, and were given in papers by Wichmann and Woo<sup>8</sup> and by Hostler.<sup>6</sup> The full Green function in momentum space had been derived in the late 1940's by Schwinger<sup>9</sup>, who made use of the explicit character of the  $SO(4)$  symmetry of the nonrelativistic hydrogen atom when it is represented in momentum space. This work was published somewhat later though. Hostler<sup>6</sup> also derived an integral representation for the radial function which has been used frequently since by several authors. In 1970 Hostler<sup>10</sup>, while examining the Coulomb Green function in  $n$ -dimensional space came across what is now referred to as the 'Sturmian' form of the radial Green function and which is basically

an infinite series of Laguerre polynomials. In the context of the phase-space formulation of the theory of the hydrogen atom Garcia-Bondia<sup>11</sup> and later Chetouani and Hamman<sup>12</sup> derived forms for the full Green-function, the latter authors giving it in terms of parabolic coordinates.

In Chapter 3 I present a self-contained analysis of both the radial and full Schrodinger-Coulomb Green functions in coordinate space. I begin by explicitly deriving the Sturmian form of the radial function directly from the defining differential equation. Then I show how it is possible to derive many other forms for the Green function appealing only to familiar properties of the various special functions involved. Thus a clear line of mathematical reasoning is shown to exist between the Sturmian form and all others.

My direct proof of the Sturmian form of the radial Schrodinger-Coulomb Green function from the defining radial equation is achieved by solving the double Laplace transform of that equation. The inverse transform, which, under general conditions is unique, gives the Sturmian form immediately. The utility of calculating matrix elements directly by taking the Laplace transform of the defining equation was reported independently by Huxtable and Hill<sup>13</sup>, Talukdar et al.<sup>14</sup>, and in the context of Lamb shift calculations by the present author<sup>15</sup>. It does not seem to have been noticed before that the same method can be used to derive a solution for the Green function itself. A by-product of this method is a direct proof of the completeness of the Sturmian wavefunctions.

The Dirac-Coulomb Green function  $G(\mathbf{r}_1, \mathbf{r}_2; z)$  is the solution (again with appropriate boundary conditions) of<sup>16</sup>



$$\left[ (\vec{\alpha} \cdot \vec{r}_1) \left[ -\frac{i\hbar c}{r_1} \frac{d}{dr_1} r_1 + \frac{ic\beta K}{r_1} \right] + \beta mc^2 - \frac{\alpha Z\hbar c}{r_1} - z \right] G(\vec{r}_1, \vec{r}_2; z) = \delta(\vec{r}_1 - \vec{r}_2). \quad (1.7)$$

The Dirac matrices  $\vec{\alpha}$  and  $\beta$  are given in Appendix A.1,  $\alpha$  is the fine-structure constant,  $c$  is the speed of light and  $K$  is the Johnson-Lippman operator defined in the next chapter. Again,  $G(r_1, r_2; z) = G^\dagger(r_2, r_1; z)$  but this time we are dealing with  $4 \times 4$  matrices so the conjugation involves a transposition. As in the nonrelativistic case there have been several different approaches to the discovery of a suitable functional form for  $G$ . These have been obviously less successful: the  $SO(4)$  symmetry is broken in the relativistic Kepler problem. Most popular has been the solution in terms of a partial wave expansion.

Apparently the first derivation of the radial Green functions was made by Wichman and Kroll<sup>17</sup> in 1956 in connection with a study of vacuum polarization effects in hydrogenic ions. Their solution, written in terms of Whittaker functions has become the standard form. Attempts at a Sturmian form appeared somewhat later in the 1970's, and were based on examination of the so-called 'Second-order Dirac equation'<sup>18</sup>. In this approach, solutions are obtained to a second-order equation from which, on application of a first-order operator the actual Dirac-Coulomb Green function can be obtained. Other authors<sup>19</sup> have reported the derivation of forms for the full Green function, but these seem to have little applicability due to their complicated nature. Common to all of these methods is the rather complicated nature of the solution. Since the standard solutions to the Dirac-Coulomb equation involve generally two different terms, the Green functions will involve four terms. This complicates somewhat the work involved in computing matrix elements.

I have been able to find a transformation of the defining radial equations for the Dirac-Coulomb Green function which allows for the formulation of the relativistic problem in a manner quite analogous to the nonrelativistic problem and which gives simple one term solutions. The method gives the radial function in Sturmian form; other forms can be obtained in precisely the same manner as is used for the radial Schrodinger-Coulomb Green function. The approach I take is closely related to the second-order theory, and to the method of solving the Dirac equation first explicitly analysed by Biedenharn<sup>20</sup> and recently revived by Su<sup>21</sup> and by Wong and Yeh<sup>22</sup> among others. None the less, my approach is sufficiently different to warrant some separate discussion. For this reason, in the next chapter I will be discussing at some length the solutions to the ordinary Schrodinger- and Dirac-Coulomb equations.

I begin Chapter 2 with a solution of the Schrodinger-Coulomb equation using Laplace transform techniques. This is more than just a warm-up exercise for the later work on the Green functions: I have found some quite straightforward derivations of the various quantum-number raising and lowering operators for both the nonrelativistic and relativistic wavefunctions, obtained in the Laplace transformed space. The treatment of the Dirac-Coulomb equation I present can be thought of as an explicit demonstration that Biedenharn's method is just a novel way of treating the two coupled radial equations which result from an entirely standard treatment of the angular part of the wavefunction. That this is so does not seem to have been previously well-appreciated. The resulting radial wavefunctions have a simple form analogous to the nonrelativistic wavefunctions. As I explained above, the real power of this approach becomes apparent when it is generalized to the solution of the Dirac-

Coulomb Green function.

The analysis of two photon processes requires the calculation of matrix elements of the Green function. Since both the nonrelativistic and relativistic wavefunctions consist essentially of exponentials multiplying polynomials (with possibly non-integral powers) once the double Laplace transforms of the Green functions are known the matrix elements follow immediately. For this reason, in Chapter 5 I present a detailed study of the double Laplace transforms, giving a variety of forms with different convergence properties. A 'generalized' Laplace transform involving spherical Bessel functions is also presented in several different forms. This transform allows for the inclusion of retardation effects into the matrix elements. In most cases forms relevant to the relativistic case are also computed. The non-integral nature of the powers in relativistic wavefunctions makes the computation of matrix elements more difficult; none the less suitable expressions can still be obtained. The results of this chapter are applied later to the analysis of two photon transitions.

To complete this presentation of the theory of the Coulomb Green functions in Chapter 6 I briefly consider the reduced Coulomb Green functions. These are of importance in perturbation theory, where the standard Green function is of no use since the energy variable  $z$  is fixed at an eigenvalue where the Green function has a pole. To overcome this difficulty the Reduced Green function  $\bar{G}(z)$  is defined by

$$\bar{G}(E) = \lim_{z \rightarrow E} [ G(z) - \sum \psi_E \psi_E^\dagger / (E - z) ] \quad (1.8)$$

where the sum is over the subspace of eigenfunctions corresponding to eigenvalue  $E$ . The Reduced Green functions can be calculated from the

definition (1.8), by a method which basically differentiates the Green function with respect to  $z$  (ref. 23), or by solving the defining differential equations. I utilize the latter method in Chapter 6, drawing heavily on the solutions already obtained for the ordinary Green function.

The Reduced Green functions are derived in Sturmian form, results which were derived in the 1970's for both the nonrelativistic<sup>24</sup> and relativistic<sup>25</sup> functions. Johnson<sup>26</sup> has presented 'closed form' expressions for the nonrelativistic radial function and Hylton<sup>27</sup> has done the same in the relativistic case. In the same chapter I show that Johnson's claim that the Sturmian forms are inconvenient for calculating matrix elements is not accurate.

## CHAPTER 2 : THE SCHRODINGER- AND DIRAC-COULOMB EQUATIONS

### 2.0 : INTRODUCTION

I begin the main part of this thesis by presenting both a non-relativistic and a relativistic treatment of the basic quantum theory of hydrogen-like atoms in the absence of external electric and magnetic fields. It is assumed that the nucleus is an infinitely heavy, spinless point charge, and thus hyperfine structure and effects due to the nuclear motion and finite size are neglected. Though this chapter will be useful for establishing notation, definitions and phase conventions, there are important reasons why what follows is more than a rehash of well-known theory.

In the first section I outline a solution of the Schrodinger-Coulomb equation using Laplace transform techniques which gives strong motivation for the methods employed in later chapters on the Green functions. I also briefly consider the solution as expressed in a parabolic coordinate system. In section two I present an approach to the Dirac-Coulomb problem quite different from that with which one might be familiar. Without recourse to the so-called second order Dirac-Coulomb equation, I show that the relativistic case can be formulated in just the same way as the nonrelativistic case. Although this work is not entirely new, previous treatments seem to have been beset with complications and misapprehensions. An understanding of the approach given here is essential to the development of the later theory on the Dirac-Coulomb Green function.

## 2.1 : THE SCHRODINGER-COULOMB EQUATION

The nonrelativistic hydrogenic eigenfunctions  $\psi_E(\mathbf{r})$  and corresponding energy eigenvalues  $E$  are found by solving the Schrodinger-Coulomb equation,

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 - \frac{\hbar^2}{amr} - E \right] \psi_E(\mathbf{r}) = 0, \quad (2.1.1)$$

subject to the boundary condition that  $\psi_E$  be a square integrable function,  $\psi_E \in L^2(\mathbb{R}^3)$ . This equation is most naturally solved by rewriting it in terms of spherical polar coordinates, in which form it is completely separable. Thus, letting

$$x = r \sin\theta \cos\phi, \quad y = r \sin\theta \sin\phi, \quad z = r \cos\theta, \quad (2.1.2)$$

the Schrodinger-Coulomb equation becomes

$$\left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left[ r^2 \frac{\partial}{\partial r} \right] - \frac{1}{r^2} \tilde{L}^2(\theta, \phi) + \frac{2}{ar} + \frac{2mE}{\hbar^2} \right] \tilde{\psi}_E(r, \theta, \phi) = 0 \quad (2.1.3)$$

where

$$\tilde{L}^2(\theta, \phi) = \frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left[ \sin\theta \frac{\partial}{\partial \theta} \right] + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \phi^2}, \quad (2.1.4)$$

and

$$\tilde{\psi}_E(r, \theta, \phi) \equiv \psi_E(r \sin\theta \cos\phi, r \sin\theta \sin\phi, r \cos\theta) \quad (2.1.5)$$

The fundamental equation we wish to solve is (2.1.1), and not (2.1.3) ; it is therefore important that we allow only those solutions  $\tilde{\psi}_E$  of (2.1.3) which lead to solutions  $\psi_E$  of (2.1.1) through (2.1.5), subject to the boundary condition. Square integrable solutions of (2.1.3) which are *not* solutions of (2.1.1) do exist; excluding such solutions leads to further restrictions on  $\tilde{\psi}_E$  <sup>28</sup>.

As the first consequence of the preceeding remarks we note that from equation (2.1.5)

$$\tilde{\psi}_E(r, \theta, \phi) = \tilde{\psi}_E(r, \theta, \phi + 2\pi) \quad (2.1.6)$$

The claim is often made that  $\tilde{\psi}_E$  must be single-valued, which also leads to the condition given in (2.1.6); from what has just been said this is *not* the basis for the restriction on the  $\phi$ -dependence of  $\tilde{\psi}_E$ .

Given this condition, together with the condition that  $\psi_E$  be normalizable, it is easy to show that we can choose

$$\tilde{\psi}_E(r, \theta, \phi) = R_{\nu\ell}(r) Y_{\ell m}(\theta, \phi) \quad (2.1.7)$$

where the  $Y_{\ell m}$ 's are spherical harmonics <sup>29</sup> (we adopt Condon and Shortley's definitions and phase conventions) and  $R_{\nu\ell}$  satisfies

$$\left[ \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{d}{dr} \right) - \frac{\ell(\ell+1)}{r^2} + \frac{2}{ar} - \frac{1}{\nu^2 a^2} \right] R_{\nu\ell}(r) = 0 \quad (2.1.8)$$

Here we have introduced the dimensionless 'generalized principal quantum number'  $\nu$ , defined by  $\nu^2 a^2 = -\hbar^2 / 2mE$ .

Given the form of the volume element in spherical polar coordinates we see that  $\psi_E$  will be square integrable if  $rR_{\nu\ell}$  is. Consequently we require that  $rR_{\nu\ell}$  approach zero rapidly enough at infinity and that it be finite at the origin. Functions which behave like  $1/r$  for small  $r$  are therefore allowed by the integrability condition. Such functions, though square integrable solutions of the radial equation, do not lead to solutions of equation (2.1.1). In fact, the Schrödinger-Coulomb operator acting on the space of such functions is non-hermitian<sup>30</sup>. It can be shown that solutions of (2.1.3) which are also solutions of (2.1.1) must behave near the origin like  $1/r^{1-\sigma}$ , where  $\sigma > 0$ , and are thus *necessarily* square integrable there.

We can now state the boundary conditions required of the solutions to equation (2.1.8) :

$$rR_{\nu\ell} \in L^2(\mathbb{R}) \quad ; \quad \lim_{r \rightarrow 0} rR_{\nu\ell}(r) = 0 \quad (2.1.9)$$

It is frequently claimed in the literature that  $R_{\nu\ell}$  must be finite at the origin ; that this is *not* the appropriate boundary condition should be clear from the above, and from the fact that the Dirac-Coulomb wavefunctions for s-states are actually singular there.

We now come to the solution of equation (2.1.8) subject to the boundary conditions (2.1.9). At this point we depart from tradition and attempt a solution utilizing Laplace transform techniques<sup>31,32</sup>, a method we will come back to when treating the Green functions. We will actually solve a more general equation, special cases of which are satisfied both by the Schrodinger- and the Dirac-Coulomb radial wavefunctions.



**THEOREM 1 :-**

The solution of

$$\left[ \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{\lambda(\lambda+1)}{r^2} + \frac{2}{\beta r} - \frac{1}{\beta^2 \nu^2} \right] f(r) = 0 \quad (2.1.10)$$

(with  $\lambda$ ,  $\beta$  and  $\nu$  positive) subject to the boundary conditions

$$rf \in L^2(\mathbb{R}) \quad \text{and} \quad \lim_{r \rightarrow 0} rf(r) = 0 \quad (2.1.11)$$

is

$$f(r) = N r^\lambda e^{-r/\beta\nu} L_{\nu-\lambda-1}^{2\lambda+1} \left[ \frac{2r}{\beta\nu} \right] \quad (2.1.12)$$

with  $\nu-\lambda-1$  a non-negative integer, and  $N$  an arbitrary constant. Here  $L_n^\alpha$  is a generalized-Laguerre polynomial as defined in Appendix A.1.

*PROOF :* We consider a related function,

$$h(r) = r^{\lambda+1} f(r) \quad (2.1.13)$$

which satisfies

$$\left[ r \frac{d^2}{dr^2} - 2\lambda \frac{d}{dr} + \frac{2}{\beta} - \frac{r}{\beta^2 \nu^2} \right] h(r) = 0 \quad (2.1.14)$$

The Laplace transform of  $h$ ,

$$H(p) = \int_0^\infty e^{-pr} h(r) dr, \quad (2.1.15)$$

satisfies the transformed equation

$$\left[ (p^2 - 1/\beta^2 \nu^2) \frac{d}{dp} + 2p(\lambda+1) - 2/\beta \right] H(p) = 0 \quad (2.1.16)$$

where we have used the fact that  $h(0) = 0$ . Finally, the function

$$G(p) = p^{2\lambda+2} H(p) \quad (2.1.17)$$

satisfies

$$\left[ (p^2 - 1/\beta^2 \nu^2) \frac{d}{dp} + \frac{2(\lambda+1)}{p\beta^2 \nu^2} - 2/\beta \right] G(p) = 0 \quad (2.1.18)$$

This equation is most easily solved if we make the change of variables

$$p \mapsto q = (p - 1/\beta\nu)/2p \quad (2.1.19)$$

so that

$$\left[ q(1-q) \frac{d}{dq} + (\lambda+1)(1-2q) - \nu \right] G(q) = 0, \quad (2.1.20)$$

which has the simple solution

$$G(q) = N'' q^{\nu-\lambda-1} (1-q)^{-\nu-\lambda-1} \quad (2.1.21)$$

Thus the Laplace transform of  $h$  is given by

$$H(p) = N' \left[ \frac{p-1/\beta\nu}{p+1/\beta\nu} \right]^\nu [(p-1/\beta\nu)(p+1/\beta\nu)]^{-\lambda-1} \quad (2.1.22)$$

$N'$  and  $N''$  are arbitrary constants.

We can immediately deduce a condition on the magnitude of  $\nu$ . If  $\nu - \lambda - 1 < 0$  then the singularity of  $H(p)$  with greatest real part is at  $p = 1/\beta\nu$ , and thus  $h(r)$  (and consequently  $f(r)$ ) will behave as  $e^{r/\beta\nu}$  as  $r$  approaches infinity<sup>31</sup>. Since this would violate the integrability condition on  $f$  we deduce that  $\nu \geq \lambda + 1$ . Now

$$\begin{aligned} H(p) &= N' \left[ 1 - \frac{2/\beta\nu}{p+1/\beta\nu} \right]^{\nu-\lambda-1} (p+1/\beta\nu)^{-2\lambda-2} \\ &= N' \sum_{n=0}^{\infty} \frac{(\lambda+1-\nu)_n}{n!} (2/\beta\nu)^n (p+1/\beta\nu)^{-2\lambda-2-n}, \end{aligned} \quad (2.1.23)$$

a series which converges absolutely for  $p > 1/\beta\nu$ . Applying a simple extension of a theorem on Laplace transforms<sup>32</sup> we can immediately deduce that

$$h(r) = N' r^{2\lambda+1} e^{-r/\beta\nu} \sum_{n=0}^{\infty} \frac{(\lambda+1-\nu)_n}{n! \Gamma(2\lambda+2+n)} \left( \frac{2r}{\beta\nu} \right)^n \quad (2.1.24)$$

Familiar arguments now can be used to show that  $h(r)$  behaves like  $e^{r/\beta\nu}$  at infinity and is therefore not square integrable unless  $\lambda+1-\nu$  is a negative integer. In view of the definition of Laguerre polynomials given in Appendix A/1 the form of  $f$  given in the theorem follows. *QED.*

Applying this theorem to equation (2.1.8), with  $\ell = \lambda$  and  $a = \beta$ , we find that since  $\nu - \ell - 1$  and  $\ell$  are integers then  $\nu$  must be an integer  $n$  with  $n \geq \ell + 1$ ; finally then

$$R_{n\ell}(r) = N_{n\ell} (2r/na)^{\ell} e^{-r/na} L_{n-\ell-1}^{2\ell+1} (2r/na) \quad (2.1.25)$$

and  $E = -\hbar^2/2ma^2n^2$ , where  $N_{n\ell}$  is chosen so as to normalize  $R$ .

The idea of solving the Schrodinger-Coulomb equation using Laplace transform techniques, though unconventional, is as unoriginal as it is possible to be; Schrodinger himself used it in his first paper on modern quantum mechanics<sup>33</sup>.

The normalization,

$$\int |\psi_E(r)|^2 d\tau = \int_0^\infty r^2 R_{n\ell}(r)^2 dr = 1, \quad (2.1.26)$$

is performed by noting that (B.1.2)

$$\int_0^\infty e^{-x} x^{\alpha+1} [L_n^\alpha(x)]^2 dx = (\alpha+1+2n) \Gamma(\alpha+1+n)/n! \quad (2.1.27)$$

so that

$$N_{n\ell} = (2/n^2 a^{3/2}) \sqrt{(n-\ell-1)!/(n+\ell)!} \quad (2.1.28)$$

An arbitrary phase factor may be introduced into the normalization constants; the only effect will be different signs in the ladder operators. The Schrodinger-Coulomb wavefunctions are thus completely determined by equations (2.1.25,28).

On purely physical grounds the separation of the Schrodinger-Coulomb equation in spherical polar coordinates is the most natural. This

separation is found to be of use whenever the angular momentum operator is conserved. But the hidden symmetry inherent in the nonrelativistic Coulomb problem, which is well known to be a consequence of the further conservation of the Runge-Lenz vector, allows for the separation of the equation in other coordinate systems. From the mathematical viewpoint the full symmetries of the Schrodinger-Coulomb equation are most vividly exposed when it is separated in parabolic coordinates<sup>34</sup>. We will perform that separation now.

The parabolic coordinate system is defined by<sup>35</sup>

$$x = \sqrt{\xi\eta} \cos\varphi, \quad y = \sqrt{\xi\eta} \sin\varphi, \quad z = (\xi - \eta)/2, \quad \text{and} \quad r = (\xi + \eta)/2 \quad (2.1.29)$$

so that the volume element is  $d\tau = (\xi + \eta)/4 \, d\xi d\eta d\varphi$ , and the Laplacian operator becomes

$$\nabla^2 = 4/(\xi + \eta) \left[ \frac{\partial}{\partial \xi} \left[ \xi \frac{\partial}{\partial \xi} \right] + \frac{\partial}{\partial \eta} \left[ \eta \frac{\partial}{\partial \eta} \right] \right] + 1/(\xi\eta) \frac{\partial^2}{\partial \varphi^2} \quad (2.1.30)$$

Thus, the Schrodinger-Coulomb equation in these coordinates,

$$\left[ \frac{\partial}{\partial \xi} \left[ \xi \frac{\partial}{\partial \xi} \right] + \frac{\partial}{\partial \eta} \left[ \eta \frac{\partial}{\partial \eta} \right] + \frac{1}{4} \left( \frac{1}{\xi} + \frac{1}{\eta} \right) \frac{\partial^2}{\partial \varphi^2} + \frac{1}{a} - \frac{(\xi + \eta)}{4a^2 \nu^2} \right] \psi_\nu(\xi, \eta, \varphi) = 0 \quad (2.1.31)$$

is clearly separable. We look for normalizable solutions of the form

$$\psi_\nu(\xi, \eta, \varphi) = e^{im\varphi} u_1(\xi) u_2(\eta) \quad (2.1.32)$$

where necessarily  $m$  is an integer. Thus (2.1.31) becomes

$$\left[ \frac{\partial}{\partial \xi} \left[ \xi \frac{\partial}{\partial \xi} \right] + \frac{\partial}{\partial \eta} \left[ \eta \frac{\partial}{\partial \eta} \right] - \frac{m^2}{4} \left[ \frac{1}{\xi} + \frac{1}{\eta} \right] + \frac{1}{a} - \frac{(\xi + \eta)}{4a^2 \nu^2} \right] u_1(\xi) u_2(\eta) = 0 \quad (2.1.33)$$

which we separate by writing

$$1/a = 1/a_1 + 1/a_2 \quad (2.1.34)$$

so that

$$\left[ \frac{d}{d\xi} \left[ \xi \frac{d}{d\xi} \right] - \frac{m^2}{4\xi} + \frac{1}{a_1} - \frac{\xi}{4a^2 \nu^2} \right] u_1(\xi) = 0 \quad (2.1.35)$$

$$\left[ \frac{d}{d\eta} \left[ \eta \frac{d}{d\eta} \right] - \frac{m^2}{4\eta} + \frac{1}{a_2} - \frac{\eta}{4a^2 \nu^2} \right] u_2(\eta) = 0 \quad (2.1.36)$$

We will content ourselves with solving in detail just the first of these two equations. Letting

$$w_1(\xi) = u_1(\xi) / \sqrt{\xi} \quad (2.1.37)$$

we find

$$\left[ \frac{d^2}{d\xi^2} + \frac{2}{\xi} \frac{d}{d\xi} + \frac{1-m^2}{4\xi^2} - \frac{1}{4a^2 \nu^2} + \frac{1}{a_1 \xi} \right] w_1(\xi) = 0 \quad (2.1.38)$$

This equation is seen to be of the same form as that solved in Theorem 1.

We may immediately state the result:

$$u_1(\xi) = N (\xi/a\nu)^{|m|/2} e^{-\xi/2a\nu} L_{n_1}^{|m|}(\xi/a\nu) \quad (2.1.39)$$

where  $n_1 = a\nu/a_1 - |m|/2 - 1/2$  is a non-negative integer. Similarly

$$u_2(\eta) = N^{1/2} (\eta/a\nu)^{|m|/2} e^{-\eta/2a\nu} L_{n_2}^{|m|}(\eta/a\nu) \quad (2.1.40)$$

with  $n_2 = a\nu/a_2 - |m|/2 - 1/2$  a non-negative integer too. In view of (2.1.34) we see that  $\nu = n = n_1 + n_2 + |m| + 1$ , a positive integer. We are thus lead back to the Bohr formula for the energy eigenvalues, with  $n$  the principal quantum number:  $E = -\hbar^2/(2ma^2n^2)$ .

The eigenfunctions in parabolic coordinates are finally given by

$$\psi_E(\xi, \eta, \varphi) = N e^{im\varphi} (\xi\eta)^{|m|/2} e^{-(\xi+\eta)/2a\nu} L_{n_1}^{|m|}(\xi/a\nu) L_{n_2}^{|m|}(\eta/a\nu) \quad (2.1.41)$$

where

$$N = (1/\sqrt{\pi n}) (a\nu)^{-|m|-3/2} \sqrt{n_1!/(n_1+|m|)!} \sqrt{n_2!/(n_2+|m|)!} \quad (2.1.42)$$

The allowed values of  $m$  are  $-n+1, \dots, n-1$ ;  $n_1$  and  $n_2$  are chosen so that  $n = n_1 + n_2 + |m| + 1$ . The normalization constant  $N$  was chosen so that

$$\int_0^\infty d\xi \int_0^\infty d\eta \int_0^{2\pi} d\varphi |\psi_E(\xi, \eta, \varphi)|^2 (\xi+\eta)/4 = 1 \quad (2.1.43)$$

and was calculated with the help of the (2.1.27) together with the following formula (B.1.6):

$$\int_0^\infty e^{-x} x^\alpha [L_n^\alpha(x)]^2 dx = \Gamma(\alpha+n+1)/n! \quad (2.1.44)$$

## 2.2 : THE DIRAC-COULOMB EQUATION

The relativistic hydrogenic eigenfunctions  $\psi_E(\vec{r})$  (which are 4-component spinors) and corresponding energy eigenvalues  $E$  are found by solving the Dirac-Coulomb equation<sup>36</sup>,

$$[ -i\hbar c \vec{\alpha} \cdot \vec{\nabla} + \beta mc^2 - \alpha Z \hbar c / r - E ] \psi_E(\vec{r}) = 0 \quad (2.2.1)$$

subject to the boundary condition that  $\psi_E^\dagger \psi_E \in L(\mathbb{R}^3)$ . (The Dirac matrices are defined in Appendix A.1.) As with the Schrodinger-Coulomb equation, the natural method of solution is in spherical polar coordinates, though some modifications are required to take into account the 4-component spinors.

Defining

$$K = \beta ( \vec{\Sigma} \cdot \vec{L}(\theta, \phi) + \hbar ) \quad (2.2.2)$$

the equation becomes

$$\left\{ (\vec{\alpha} \cdot \vec{r}) \left[ -\frac{i\hbar c}{r} \frac{\partial}{\partial r} r + \frac{ic}{r} \beta K \right] + \beta mc^2 - \frac{\alpha Z}{r} - E \right\} \times \tilde{\psi}_E(r, \theta, \phi) = 0 \quad (2.2.3)$$

where

$$\tilde{\psi}_E(r, \theta, \phi) \equiv \psi_E(r \sin\theta \cos\phi, r \sin\theta \sin\phi, r \cos\phi) \quad (2.2.4)$$



The total angular momentum operator,

$$\vec{J}(\theta, \phi) = \vec{L}(\theta, \phi) + \hbar/2 \vec{\Sigma} \quad (2.2.5)$$

and  $K$  commute with the Dirac-Coulomb operator; we may thus look for solutions to (2.2.3) which are eigenfunctions of  $\vec{J}^2$ ,  $J_z$  and  $K$ , with eigenvalues  $\hbar^2 j(j+1)$ ,  $\hbar M$  and  $-\hbar\kappa$  respectively. The allowed values, given the boundary conditions, are:  $j = 1/2, 3/2, \dots$ ;  $M = -j, -j+1, \dots, +j$ ;  $\kappa = \pm (j+1/2)$ .

The solution of (2.2.3) is now found to be of the form<sup>36</sup>

$$\tilde{\psi}_E(r, \theta, \phi) = \begin{bmatrix} f_1(r) \chi_\kappa^M(\theta, \phi) \\ if_2(r) \chi_{-\kappa}^M(\theta, \phi) \end{bmatrix} \quad (2.2.6)$$

where

$$\chi_\kappa^M(\theta, \phi) = \begin{bmatrix} \frac{-\kappa}{|\kappa|} \left[ \frac{\kappa+1/2-M}{2\kappa+1} \right]^{\frac{1}{2}} Y_{|\kappa+\frac{1}{2}|-\frac{1}{2}, M-\frac{1}{2}}(\theta, \phi) \\ \left[ \frac{\kappa+1/2+M}{2\kappa+1} \right]^{\frac{1}{2}} Y_{|\kappa+\frac{1}{2}|-\frac{1}{2}, M+\frac{1}{2}}(\theta, \phi) \end{bmatrix} \quad (2.2.7)$$

and the radial wavefunctions satisfy

$$\left[ mc^2 - \frac{\alpha Z \hbar c}{r} - E \right] f_1(r) + \left[ \frac{\hbar c \kappa}{r} - \frac{\hbar c}{r} \frac{d}{dr} r \right] f_2(r) = 0, \quad (2.2.8a)$$

$$\left[ \frac{\hbar c}{r} \frac{d}{dr} r + \frac{\hbar c \kappa}{r} \right] f_1(r) - \left[ mc^2 + \frac{\alpha Z \hbar c}{r} + E \right] f_2(r) = 0. \quad (2.2.8b)$$

The  $\chi$ 's are normalized so that

$$\int_0^\pi \int_0^{2\pi} \chi_\kappa^M(\theta, \phi)^\dagger \chi_{\kappa'}^{M'}(\theta, \phi) \sin\theta \, d\theta d\phi = \delta_{\kappa, \kappa'} \delta_{M, M'} \quad (2.2.9)$$

The integrability condition on  $\psi_E$  now implies that  $|f_1|$  and  $|f_2|$  be square integrable, and this is the main boundary condition we employ in solving (2.2.8). In fact,

$$\int \psi_E(r)^\dagger \psi_E(r) \, dr = \int (|f_1(r)|^2 + |f_2(r)|^2) r^2 \, dr \quad (2.2.10)$$

We now come to the solution of the two radial equations. At this point we depart from tradition again by showing how a simple transformation of the two functions can be found which reduces the solution to the nonrelativistic one. We begin by defining

$$\epsilon = E/\hbar c \quad , \quad \epsilon_0 = mc^2/\hbar c \quad (2.2.11)$$

so that equations (2.2.8) become

$$\left[ \epsilon_0 - \epsilon - \frac{\alpha Z}{r} \right] f_1(r) + \left[ -\frac{d}{dr} + \frac{\kappa-1}{r} \right] f_2(r) = 0 \quad (2.2.12a)$$

$$\left[ \frac{d}{dr} + \frac{\kappa+1}{r} \right] f_1(r) - \left[ \epsilon_0 + \epsilon + \frac{\alpha Z}{r} \right] f_2(r) = 0 \quad (2.2.12b)$$

We now introduce two related functions,  $g_1$  and  $g_2$ , defined by

$$g_1 = f_1 + \kappa f_2 \quad , \quad g_2 = \kappa f_1 + f_2 \quad (2.2.13)$$

so that

$$f_1 = (1-N^2)^{-1}(g_1 - Ng_2) , \quad f_2 = (1-N^2)^{-1}(-Ng_1 + g_2) , \quad (2.2.14)$$

where the constant  $N$  is to be determined. These functions satisfy

$$\begin{aligned} & \left[ (\epsilon_0 - \epsilon) - \frac{\alpha Z + N\kappa - N}{r} + N \frac{d}{dr} \right] g_1(r) \\ & + \left[ -N(\epsilon_0 - \epsilon) + \frac{N\alpha Z + \kappa - 1}{r} - \frac{d}{dr} \right] g_2(r) = 0 \end{aligned} \quad (2.2.15a)$$

$$\begin{aligned} & \left[ N(\epsilon_0 + \epsilon) + \frac{N\alpha Z + \kappa + 1}{r} + \frac{d}{dr} \right] g_1(r) \\ & - \left[ (\epsilon_0 + \epsilon) + \frac{\alpha Z + N\kappa + N}{r} + N \frac{d}{dr} \right] g_2(r) = 0 , \end{aligned} \quad (2.2.15b)$$

and, on eliminating a derivative from each equation in turn,

$$\begin{aligned} & \left[ \epsilon_0(1-N^2) - \epsilon(1+N^2) - \frac{\alpha Z(1+N^2) + 2N\kappa}{r} \right] g_1(r) \\ & + \left[ 2N\epsilon + \frac{2N\alpha Z + (1+N^2)\kappa - (1-N^2)}{r} - (1-N^2) \frac{d}{dr} \right] g_2(r) = 0 , \end{aligned} \quad (2.2.16a)$$

$$\begin{aligned} & \left[ 2N\epsilon + \frac{2N\alpha Z + (1+N^2)\kappa + (1-N^2)}{r} + (1-N^2) \frac{d}{dr} \right] g_1(r) \\ & - \left[ \epsilon_0(1-N^2) + \epsilon(1+N^2) + \frac{\alpha Z(1+N^2) + 2N\kappa}{r} \right] g_2(r) = 0 . \end{aligned} \quad (2.2.16b)$$

Quite remarkably, if we now choose

$$N = (-\kappa + \chi)/\alpha Z \quad (2.2.17)$$

where  $\gamma = \sqrt{\kappa^2 - \alpha^2 Z^2}$ , one term in each of the two equations drops out, and we are left with

$$\left[ \epsilon_0 - \frac{\epsilon \kappa}{\gamma} \right] g_1(r) + \left[ -\frac{\alpha Z \epsilon}{\gamma} + \frac{\gamma-1}{r} - \frac{d}{dr} \right] g_2(r) = 0, \quad (2.2.18a)$$

$$\left[ -\frac{\alpha Z \epsilon}{\gamma} + \frac{\gamma+1}{r} + \frac{d}{dr} \right] g_1(r) - \left[ \epsilon_0 + \frac{\epsilon \kappa}{\gamma} \right] g_2(r) = 0. \quad (2.2.18b)$$

Finally, we eliminate  $g_1$  and  $g_2$  in turn from the equations to arrive at the form we desire:

$$\left[ \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{\gamma(\gamma+1)}{r^2} + \frac{2\alpha Z \epsilon}{r} + \epsilon^2 - \epsilon_0^2 \right] g_1(r) = 0; \quad (2.2.19a)$$

$$\left[ \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{(\gamma-1)\gamma}{r^2} + \frac{2\alpha Z \epsilon}{r} + \epsilon^2 - \epsilon_0^2 \right] g_2(r) = 0. \quad (2.2.19b)$$

Since  $L^2(\mathbb{R})$  is a linear space the boundary conditions on  $g_1$  and  $g_2$  are the same as those on  $f_1$  and  $f_2$ . Thus:

$$r g_1, r g_2 \in L^2(\mathbb{R}) \quad ; \quad \lim_{r \rightarrow 0} r g_1(r), r g_2(r) = 0. \quad (2.2.20)$$

It is immediately clear that the solutions of equations (2.2.19) have been already found in THEOREM 1. The solutions are

$$g_1(r) = N_1 (2r\sqrt{\epsilon_0^2 - \epsilon^2})^\gamma e^{-r\sqrt{\epsilon_0^2 - \epsilon^2}} L_{N-1}^{2\gamma+1} (2r\sqrt{\epsilon_0^2 - \epsilon^2}), \quad (2.2.21)$$

$$g_2(r) = N_2 (2r\sqrt{\epsilon_0^2 - \epsilon^2})^{\gamma-1} e^{-r\sqrt{\epsilon_0^2 - \epsilon^2}} L_N^{2\gamma-1} (2r\sqrt{\epsilon_0^2 - \epsilon^2}). \quad (2.2.22)$$

Here,

$$N = \alpha Z \epsilon / \sqrt{\epsilon_0^2 - \epsilon^2} - \gamma \quad (2.2.23)$$

is necessarily an integer, and this leads immediately to the well-known expression for the relativistic energy eigenvalues:

$$E = mc^2 / [1 + \alpha^2 Z^2 / (N + \gamma)^2]^{\frac{1}{2}} \quad (2.2.24)$$

(The negative root would render  $N$  negative and is therefore not applicable.)

Some care is required in calculating the normalization constants,  $N_1$  and  $N_2$ . Consideration of equation (2.2.18b) at  $r=0$  leads to the following relationship between the two constants:

$$N(2\gamma + N)\sqrt{\epsilon_0^2 - \epsilon^2} N_1 = (\epsilon\kappa + \epsilon_0\gamma) N_2 \quad (2.2.25)$$

Their absolute values are fixed by the normalization condition,

$$\begin{aligned} \int \psi_E(\vec{r})^\dagger \psi_E(\vec{r}) d\vec{r} &= 1 \\ &= \int_0^\infty [f_1(r)^2 + f_2(r)^2] r^2 dr \\ &= \frac{\kappa(\kappa + \gamma)}{2\gamma^2} \int_0^\infty [g_1(r)^2 + \frac{2\alpha Z}{\kappa} g_1(r)g_2(r) + g_2(r)^2] r^2 dr \quad (2.2.26) \end{aligned}$$

The integrals in (2.2.26) can be easily performed; we simply use (2.1.17) again, and the following Laplace transform which is proved in Appendix B.1:

$$\int_0^\infty e^{-x} x^{\alpha+1} L_n^{\alpha-1}(x) L_{n-1}^{\alpha+1}(x) dx = -2\Gamma(\alpha+n+1)/(n-1)! \quad (2.2.27)$$

Substituting our solutions for  $g_1$  and  $g_2$  into (2.2.26) gives

$$\frac{\kappa(\kappa+\gamma)\Gamma(2\gamma+N)}{8\gamma^2 N! \sqrt{\epsilon_0^2 - \epsilon^2}} \left[ (\gamma+N)(2\gamma+N)NN_1^2 - \frac{2\alpha Z}{\kappa}(2\gamma+N)NN_1N_2 + (\gamma+N)N_2^2 \right] = 1 \quad (2.2.28)$$

writing  $N_1$  in terms of  $N_2$ , and eliminating  $N$  from the term in square brackets noting (2.2.23) and

$$N(N+2\gamma) = (\kappa\epsilon - \gamma\epsilon_0)(\kappa\epsilon + \gamma\epsilon_0)/(\epsilon_0^2 - \epsilon^2) \quad (2.2.29)$$

leads us finally to

$$N_2 = 2(\epsilon_0^2 - \epsilon^2)/(\epsilon_0 \sqrt{\alpha Z}) [N! (\kappa\epsilon - \gamma\epsilon_0)/(\Gamma(2\gamma+N)(\kappa+\gamma))]^{\frac{1}{2}}, \quad (2.2.30)$$

$$N_1 = \left| \frac{\kappa}{|\kappa|} \right| 2(\epsilon_0^2 - \epsilon^2)^{3/2}/(\epsilon_0 \sqrt{\alpha Z}) [N! / (\Gamma(2\gamma+N)(\kappa+\gamma)(\kappa\epsilon - \gamma\epsilon_0))]^{\frac{1}{2}}. \quad (2.2.31)$$

The solution when  $N=0$  requires special consideration. Clearly  $N_1$  must vanish, otherwise the 'Laguerre polynomial'  $L_{-1}^{2\gamma+1}$ , thought of as a hypergeometric function will be non-terminating and therefore will not satisfy the boundary conditions. When  $N=0$  the energy is given by  $\epsilon(0) = \epsilon_0 \gamma/|\kappa|$  and consequently  $(\kappa\epsilon + \gamma\epsilon_0) = \epsilon_0 \gamma(\kappa+|\kappa|)/|\kappa|$ . Thus for positive  $\kappa$ , equation (2.2.25) implies that  $N_2 = 0$  and the eigenfunction vanishes identically. In this case then, only negative values of  $\kappa$  are allowed. The normalisation constants are then given by

$$N_1 = 0 ,$$

$$N_2 = 4\gamma(\epsilon_0 \alpha Z/|\kappa|)^{3/2}/\sqrt{\Gamma(2\gamma+1)\kappa(\kappa+\gamma)} \quad (2.2.32)$$

This completes the solution of the Dirac-Coulomb equation.

It is instructive to examine more closely the relationship between the radial wavefunctions we have just computed, and the physical radial wavefunctions it was our original aim to derive. Noting that

$$R = -(\kappa/|\kappa|)\sqrt{(\kappa-\gamma)/(\kappa+\gamma)} , \quad 1-R^2 = 2\gamma/(\kappa+\gamma) \quad (2.2.33)$$

we can express (2.2.14) in terms of the total angular momentum  $j$  and  $\gamma$ .

Thus, when  $\kappa = (j+1/2)$  we find

$$f_1 = (\sqrt{j+1/2+\gamma} g_1 + \sqrt{j+1/2-\gamma} g_2) \sqrt{j+1/2+\gamma} / 2\gamma , \quad (2.2.34)$$

$$f_2 = (\sqrt{j+1/2-\gamma} g_1 + \sqrt{j+1/2+\gamma} g_2) \sqrt{j+1/2+\gamma} / 2\gamma ;$$

and when  $\kappa = -(j+1/2)$

$$f_1 = -(\sqrt{j+1/2-\gamma} g_1 - \sqrt{j+1/2+\gamma} g_2) \sqrt{j+1/2-\gamma} / 2\gamma , \quad (2.2.35)$$

$$f_2 = (\sqrt{j+1/2+\gamma} g_1 - \sqrt{j+1/2-\gamma} g_2) \sqrt{j+1/2-\gamma} / 2\gamma .$$

Notice that interchanging  $g_1$  and  $g_2$  in both cases simply interchanges  $f_1$  and  $f_2$ . In view of the standard representations for the Dirac-Coulomb wavefunctions our result is seen to be in a particularly simple form. Perhaps the most interesting consequence of our solutions is that they admit

of an exceedingly straightforward treatment in the nonrelativistic limit. In fact, in the limit as  $\alpha Z \rightarrow 0$  only one or other of  $g_1$  and  $g_2$  contributes in equations (2.2.34,35) and their contribution is transparently the Schrodinger-Coulomb wavefunction. This I will now demonstrate.

As is well-known, the nonrelativistic limit is equivalent to the limit as  $\alpha Z \rightarrow 0$ ; it is important to note, however that  $\epsilon_0$  is not independent of  $\alpha Z$ . In fact  $\epsilon_0 \alpha Z = 1/a$ , where  $a$  is as before the atomic radius. For reference I will now write down the various factors occurring in the wavefunctions given to lowest order in  $\alpha Z$ .

$$\sqrt{\epsilon_0^2 - \epsilon^2} \simeq 1/a(N+|\kappa|), \quad \gamma \simeq |\kappa|, \quad |\kappa| + \gamma \simeq 2|\kappa|, \quad |\kappa| - \gamma \simeq \alpha^2 Z^2 / (2|\kappa|),$$

$$|\kappa| \epsilon + \gamma \epsilon_0 \simeq 2|\kappa| / (a \alpha Z), \quad |\kappa| \epsilon - \gamma \epsilon_0 \simeq N(N+2|\kappa|) \alpha Z / [2a|\kappa|(N+|\kappa|)^2] \quad (2.2.36)$$

and  $|\kappa|^2 - \gamma^2 = \alpha^2 Z^2$  exactly.

For  $\kappa = |\kappa|$ , equations (2.2.34) become

$$f_1 \simeq g_1 + \alpha Z / 2|\kappa| g_2; \quad f_2 \simeq \alpha Z / 2|\kappa| g_1 + g_2 \quad (2.2.37)$$

and

$$N_1 \simeq 2 / [a^{3/2}(N+|\kappa|)^2] \sqrt{(N-1)! / (2|\kappa|+N)!}$$

$$N_2 \simeq N(N+2|\kappa|) / [a^{3/2}|\kappa|(N+|\kappa|)^3] \sqrt{(N-1)! / (2|\kappa|+N)!} (\alpha Z)^{-1/2} \quad (2.2.38)$$

Thus to lowest order



$$f_1(r) = \sqrt{\frac{(N-1)!}{(2|\kappa|+N)!}} \left[ \frac{2r}{a(N+|\kappa|)} \right]^{|\kappa|} \frac{2e^{-r/a(N+|\kappa|)}}{a^{3/2}(N+|\kappa|)^2} L_{N-1}^{2|\kappa|+1} \left[ \frac{2r}{a(N+|\kappa|)} \right],$$

$$f_2(r) = 0 \quad (2.2.39)$$

Examination of the angular part of the wavefunctions shows that we may put  $|\kappa|=\ell$ , and  $N=n-\ell$  where  $n$  and  $\ell$  are the nonrelativistic quantum numbers. Thus, in the nonrelativistic limit  $f_1(r) = R_{n\ell}(r)$  and  $f_2(r) = 0$ , as we would expect.

In the case when  $\kappa=-|\kappa|$  we proceed in an exactly similar manner. This time  $g_2$  survives:

$$f_1 = -\alpha^2 Z^2 / 4 |\kappa|^2 g_1 + \alpha Z / 2 |\kappa| g_2, \quad f_2 = \alpha Z / 2 |\kappa| g_1 - \alpha^2 Z^2 / 4 |\kappa|^2 g_2, \quad (2.2.40)$$

leads immediately to

$$f_1(r) = \sqrt{\frac{N!}{(2|\kappa|+N-1)!}} \left[ \frac{2r}{a(N+|\kappa|)} \right]^{|\kappa|-1} \frac{2e^{-r/a(N+|\kappa|)}}{a^{3/2}(N+|\kappa|)^2} L_N^{2|\kappa|-1} \left[ \frac{2r}{a(N+|\kappa|)} \right],$$

$$f_2(r) = 0. \quad (2.2.41)$$

Putting now  $|\kappa|=\ell+1$  and  $N=n-\ell-1$  gives the expected result once again:  $f_1(r) = R_{n\ell}(r)$  and  $f_2(r) = 0$ .

This now completes our brief, if unconventional survey of the Dirac-Coulomb equation. The solutions given above have been derived before in what seems to me to be less natural treatments. The method is closely related to the treatment utilizing the second order Dirac equation;

the latter method treats the entire equation however, whereas I have shown that the radial equations are all that we have to solve in a non-standard manner. Biedenharn<sup>20</sup> and later Wong and Yeh<sup>22</sup> and Su<sup>21</sup> solved the ordinary Dirac equation in a non-standard manner, but again their treatment involves the entire Dirac equation. The preceding solution seems to be preferable in view of its manifest transparency.

### 2.3 : RECURSION RELATIONS AND OTHER PROPERTIES OF THE COULOMB RADIAL WAVEFUNCTIONS.

We have seen through our proof of THEOREM 1 that the Laplace transform,  $\mathcal{L}[r^{\lambda+1} f_{\nu\lambda}(r, \beta)](p)$ , where

$$f_{\nu\lambda}(r, \beta) = (\nu - \lambda - 1)! / \Gamma(\nu + \lambda + 1) r^\lambda e^{-r/\beta\nu} L_{\nu-\lambda-1}^{2\lambda+1}(2r/\beta\nu) \quad (2.3.1)$$

is

$$S_{\nu\lambda}(p; \beta) = \left[ \frac{p-1/\beta\nu}{p+1/\beta\nu} \right]^\nu 1/(p^2-1/\beta^2\nu^2)^{\lambda+1}, \quad (2.3.2)$$

and satisfies

$$\left[ (p^2-1/\beta^2\nu^2) \frac{d}{dp} + 2p(\lambda+1) - 2/\beta \right] S_{\nu\lambda}(p; \beta) = 0 \quad (2.3.3)$$

The particularly simple form of  $S$  allows us to quickly derive various raising and lowering operators for  $\lambda$  and  $\nu$  which will, in turn lead to raising and lowering operators of  $f$ .

From (2.3.2) we see immediately that

$$(p^2-1/\beta^2\nu^2) S_{\nu\lambda}(p; \beta) = S_{\nu\lambda-1}(p; \beta) \quad (2.3.4)$$

which is a lowering operator for  $\lambda$ . Let us now differentiate (2.3.4) with respect to  $p$ . Then

$$\begin{aligned}
\frac{d}{dp} S_{\nu\lambda-1}(p;\beta) &= \frac{d}{dp} ((p^2-1/\beta^2\nu^2)S_{\nu\lambda}(p;\beta)) \\
&= (p^2-1/\beta^2\nu^2) \frac{d}{dp} S_{\nu\lambda}(p;\beta) + 2pS_{\nu\lambda}(p;\beta) \\
&= [2/\beta - 2p(\lambda+1)] S_{\nu\lambda}(p;\beta) + 2pS_{\nu\lambda}(p;\beta) \\
&= -2(\lambda p - 1/\beta) S_{\nu\lambda}(p;\beta) ,
\end{aligned}$$

where we have made use of (2.3.3) at the third step. Now, taking note of (2.3.4) again we have

$$\begin{aligned}
(\lambda p + 1/\beta) \frac{d}{dp} S_{\nu\lambda-1}(p;\beta) &= -2(\lambda^2 p^2 - 1/\beta^2) S_{\nu\lambda}(p;\beta) \\
&= -2\lambda^2 [ 1/\beta^2 \nu^2 S_{\nu\lambda}(p;\beta) + S_{\nu\lambda-1}(p;\beta) ] + 2/\beta^2 S_{\nu\lambda}(p;\beta) ,
\end{aligned}$$

giving finally the following raising operator for  $\lambda$  :

$$\left[ (\lambda p + 1/\beta) \frac{d}{dp} + 2\lambda^2 \right] S_{\nu\lambda-1}(p;\beta) = \frac{2}{\beta^2} \left[ \frac{\nu^2 - \lambda^2}{\nu^2} \right] S_{\nu\lambda}(p;\beta) . \quad (2.3.5)$$

The raising and lowering operators for  $\nu$  are only slightly more complicated. From (2.3.2) we see that

$$(p+1/\beta\nu) S_{\nu\lambda}(p;\beta) = \left[ \frac{\nu}{\nu-1} \right]^{2\lambda+2} (p-1/\beta\nu) S_{\nu-1\lambda} \left[ \frac{\nu}{\nu-1} p; \beta \right] \quad (2.3.6)$$

and this equation, together with (2.3.4) implies

$$S_{\nu\lambda-1}(p;\beta) = \left[ \frac{\nu}{\nu-1} \right]^{2\lambda+2} (p-1/\beta\nu)^2 S_{\nu-1\lambda} \left[ \frac{\nu}{\nu-1} p; \beta \right] , \quad (2.3.7)$$

$$(p+1/\beta\nu)^2 S_{\nu\lambda}(p;\beta) = \left[ \frac{\nu}{\nu-1} \right]^{2\lambda} S_{\nu-1\lambda-1} \left[ \frac{\nu}{\nu-1} p; \beta \right] . \quad (2.3.8)$$

The plan is now to raise the  $\lambda-1$  to  $\lambda$  in (2.3.7) and (2.3.8) making use of (2.3.5), this being facilitated by the fact that the differential operator does not depend on  $\nu$ . Beginning with (2.3.7) we find

$$\frac{2}{\beta} \left[ \frac{\nu^2 - \lambda^2}{\nu^2} \right] S_{\nu\lambda}(p; \beta) = \left[ \frac{\nu}{\nu-1} \right]^{2\lambda+2} \left[ (p-1/\beta\nu)^2 \left( (p+1/\beta) \frac{d}{dp} + 2\lambda^2 \right) + 2(p-1/\beta\nu)(\lambda p+1/\beta) \right] S_{\nu-1\lambda} \left[ \frac{\nu}{\nu-1} p; \beta \right]$$

We now make repeated use of (2.3.3) to reduce terms in  $p^3 d/dp$  and  $p^2 d/dp$  to terms at most of the form  $p d/dp$ . Then we arrive at a  $\nu$  raising operator:

$$\left[ (\nu-\lambda-1) - (p-1/\beta\nu) \frac{d}{dp} \right] S_{\nu\lambda}(p; \beta) = (\nu+\lambda+1) \left[ \frac{\nu}{\nu+1} \right]^{2\lambda+2} S_{\nu+1\lambda} \left[ \frac{\nu}{\nu+1} p; \beta \right] \quad (2.3.9)$$

The same procedure applied to (2.3.8) gives a  $\nu$  lowering operator just as quickly:

$$\left[ (\nu+\lambda+1) + (p+1/\beta\nu) \frac{d}{dp} \right] S_{\nu\lambda}(p; \beta) = (\nu-\lambda-1) \left[ \frac{\nu}{\nu-1} \right]^{2\lambda+2} S_{\nu-1\lambda} \left[ \frac{\nu}{\nu-1} p; \beta \right] \quad (2.3.10)$$

Both (2.3.9) and (2.3.10) can be checked directly given the simple algebraic form of  $S$ .

Notice that all the equations we have presented in this section were derived either from the form of  $S$  or from it's defining equation. We can of course, take the inverse Laplace transforms to get ladder operators for  $f_{\nu\lambda}$ . The only difficulty encountered in this is the treatment of the  $p^2$

term in (2.3.4) which leads to a term in  $d^2/dr^2$  on inverting the equation. This can be easily dealt with by using the differential equation satisfied by  $f_{\nu\lambda}$ :

$$\left[ \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{\lambda(\lambda+1)}{r^2} + \frac{2}{\beta r} - \frac{1}{\beta^2 \nu^2} \right] f_{\nu\lambda}(r, \beta) = 0 \quad (2.3.11)$$

(see (2.1.10)). The ladder operators for  $f_{\nu\lambda}$  are then given by:

$$\left[ \lambda \left[ \frac{d}{dr} + \frac{\lambda+1}{r} \right] - 1/\beta \right] f_{\nu\lambda}(r, \beta) = 1/2 f_{\nu\lambda-1}(r, \beta) ; \quad (2.3.12)$$

$$\left[ \lambda \left[ \frac{d}{dr} - \frac{\lambda-1}{r} \right] + 1/\beta \right] f_{\nu\lambda-1}(r, \beta) = - \frac{2}{\beta^2} \left[ \frac{\nu^2 - \lambda^2}{\nu^2} \right] f_{\nu\lambda}(r, \beta) ; \quad (2.3.13)$$

$$\left[ (\nu+1) + r \left[ \frac{d}{dr} - 1/\beta\nu \right] \right] f_{\nu\lambda}(r, \beta) = (\nu+\lambda+1) \left[ \frac{\nu}{\nu+1} \right]^\lambda f_{\nu+1\lambda} \left[ \frac{\nu+1}{\nu} r, \beta \right] ; \quad (2.3.14)$$

$$\left[ (\nu-1) - r \left[ \frac{d}{dr} + 1/\beta\nu \right] \right] f_{\nu\lambda}(r, \beta) = (\nu-\lambda-1) \left[ \frac{\nu}{\nu-1} \right]^\lambda f_{\nu-1\lambda} \left[ \frac{\nu-1}{\nu} r, \beta \right] . \quad (2.3.15)$$

We can now apply these ladder operators to the Schrodinger-Coulomb wavefunctions (in both spherical polar and parabolic coordinates) and to the Dirac-Coulomb wavefunctions. We begin with the radial Schrodinger-Coulomb wavefunctions. Since

$$f_{n\ell}(r; a) = (-1)^{n-\ell-1} (n^2 a^{3/2})/2 (an/2)^\ell \sqrt{(n-\ell-1)!/(n+\ell)!} R_{n\ell}(r) ,$$

we have the following relationships<sup>34</sup>:

$$\left[ \ell \left[ \frac{d}{dr} + \frac{\ell+1}{r} \right] - 1/a \right] R_{n\ell}(r) = -1/a \sqrt{1-\ell^2/n^2} R_{n\ell-1}(r) ; \quad (2.3.16)$$

$$\left[ \ell \left[ \frac{d}{dr} - \frac{\ell-1}{r} \right] + 1/a \right] R_{n\ell-1}(r) = 1/a \sqrt{1-\ell^2/n^2} R_{n\ell}(r) ; \quad (2.3.17)$$

$$\left[ (n+1) + r \left[ \frac{d}{dr} - 1/an \right] \right] R_{n\ell}(r) = \left[ \frac{n+1}{n} \right]^2 \sqrt{(n-\ell)(n+\ell+1)} R_{n+1\ell} \left[ \frac{n+1}{n} r \right] ; \quad (2.3.18)$$

$$\left[ (n-1) - r \left[ \frac{d}{dr} + 1/an \right] \right] R_{n\ell}(r) = \left[ \frac{n-1}{n} \right]^2 \sqrt{(n+\ell)(n-\ell-1)} R_{n-1\ell} \left[ \frac{n-1}{n} r \right] . \quad (2.3.19)$$

Rather than labouring the point by writing down similar operators for the wavefunctions in parabolic coordinates,  $u_1^{n_1 m}(\xi)$  and  $u_2^{n_2 m}(\eta)$ , we move straight on to the relativistic case. In this case we have to be clear to distinguish normalization constants for different values of  $N$ . We begin by noting that

$$f_{N+\gamma, \gamma}(r; 1/\alpha Z \epsilon_N) = \frac{(N-1)!}{\Gamma(2\gamma+N+1)} \frac{1}{[N_1^{N\kappa} (2\sqrt{\epsilon_0^2 - \epsilon_N^2})^\gamma]} g_1^{N\kappa}(r) ,$$

$$f_{N+\gamma, \gamma-1}(r; 1/\alpha Z \epsilon_N) = \frac{N!}{\Gamma(2\gamma+N)} \frac{1}{[N_2^{N\kappa} (2\sqrt{\epsilon_0^2 - \epsilon_N^2})^{\gamma-1}]} g_2^{N\kappa}(r) ,$$

from which, noting (2.2.25) we find that (2.3.12) becomes

$$\left[ \gamma \left[ \frac{d}{dr} + \frac{\gamma+1}{r} \right] - \alpha Z \epsilon_N \right] g_1^{N\kappa}(r) = (\epsilon_N \kappa + \epsilon_0 \gamma) g_2^{N\kappa}(r) , \quad (2.3.20)$$

which is just equation (2.2.18b), and (2.3.13) becomes

$$\left[ \gamma \left[ \frac{d}{dr} - \frac{\gamma-1}{r} \right] + \alpha Z \epsilon_N \right] g_2^{N\kappa}(r) = -(\epsilon_N \kappa - \epsilon_0 \gamma) g_1^{N\kappa}(r) , \quad (2.3.21)$$

which is equation (2.2.18a). Notice that the  $\lambda$ -raising and -lowering operators do not change  $\kappa$ , which appears under a root sign in  $\gamma$  and is thus inaccessible; rather they interchange the roles of  $g_1$  and  $g_2$ . These recursion relations were first noted by Biedenharn<sup>20</sup>.

The  $\nu$ -raising and -lowering operators appear in a somewhat more complicated form. We content ourselves with presenting the results:

$$\begin{aligned} \left[ (N+\gamma+1) + r \left[ \frac{d}{dr} - \sqrt{\epsilon_0^2 - \epsilon_N^2} \right] \right] g_1^{N\kappa}(r) \\ = \sqrt{N(N+1+2\gamma)} B_{N\kappa}^2 D_{N\kappa} g_1^{N+1\kappa}(r C_{N\kappa}) \end{aligned} \quad (2.3.22)$$

$$\begin{aligned} \left[ (N+\gamma+1) + r \left[ \frac{d}{dr} - \sqrt{\epsilon_0^2 - \epsilon_N^2} \right] \right] g_2^{N\kappa}(r) \\ = (N+2\gamma) \sqrt{N/(N+1+2\gamma)} B_{N\kappa}^3 / D_{N\kappa} g_2^{N+1\kappa}(r C_{N\kappa}) \end{aligned} \quad (2.3.23)$$

$$\begin{aligned} \left[ (N+\gamma-1) - r \left[ \frac{d}{dr} + \sqrt{\epsilon_0^2 - \epsilon_N^2} \right] \right] g_1^{N\kappa}(r) \\ = \sqrt{(N-1)(N+2\gamma)} 1/(B_{N-1\kappa}^2 D_{N-1\kappa}) g_1^{N-1\kappa}(r/C_{N-1\kappa}) \end{aligned} \quad (2.3.24)$$

$$\begin{aligned} \left[ (N+\gamma-1) - r \left[ \frac{d}{dr} + \sqrt{\epsilon_0^2 - \epsilon_N^2} \right] \right] g_2^{N\kappa}(r) \\ = N \sqrt{(N+2\gamma)/(N-1)} D_{N-1\kappa} / B_{N-1\kappa}^3 g_2^{N-1\kappa}(r/C_{N-1\kappa}) \end{aligned} \quad (2.3.25)$$

where  $B_{N\kappa} = (\epsilon_N/\epsilon_{N+1})^{(N+1+\gamma)/(N+\gamma)}$ ,

$$D_{N\kappa} = [(\kappa\epsilon_N + \gamma\epsilon_0)/(\kappa\epsilon_{N+1} + \gamma\epsilon_0)]^{1/2} \quad \text{and} \quad C_{N\kappa} = [(\epsilon_0^2 - \epsilon_N^2)/(\epsilon_0^2 - \epsilon_{N+1}^2)]^{1/2}. \quad (2.3.26)$$

It is interesting to note that the last four recursion relations can be easily



shown to reduce to the nonrelativistic ones in the limit  $\alpha Z \rightarrow 0$ . I have been unable to find any reference to these last recursion relations in the literature.

We end this section with presenting some results, which will be of use in the later chapters on the Green functions. By considering the function

$$f_{k+\lambda+1,\lambda}(r, \beta\nu/(k+\lambda+1)) = \frac{k!}{\Gamma(2\lambda+2+k)} r^\lambda e^{-r/\beta\nu} L_k^{2\lambda+1}(2r/\beta\nu) \quad (2.3.27)$$

where  $k$  is an integer, and rearranging equations (2.3.11,12,13), we can derive the following formulae:

$$\left[ \frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} - \frac{\lambda(\lambda+1)}{r^2} + \frac{2}{\beta r} - \frac{1}{\beta^2 \nu^2} \right] \left[ r^\lambda e^{-r/\beta\nu} L_k^{2\lambda+1}(2r/\beta\nu) \right] \\ = -2/\beta\nu (k+\lambda+1-\nu) r^{\lambda-1} e^{-r/\beta\nu} L_k^{2\lambda+1}(2r/\beta\nu); \quad (2.3.28)$$

$$\left[ \lambda \left[ \frac{d}{dr} + \frac{\lambda+1}{r} \right] - 1/\beta \right] \left[ r^\lambda e^{-r/\beta\nu} L_k^{2\lambda+1}(2r/\beta\nu) \right] \\ = (k+\lambda+1-\nu)/\beta\nu r^\lambda e^{-r/\beta\nu} L_k^{2\lambda+1}(2r/\beta\nu) \\ + (k+1)(2\lambda+k+1)/2 r^{\lambda-1} e^{-r/\beta\nu} L_{k+1}^{2\lambda-1}(2r/\beta\nu); \quad (2.3.29)$$

$$\left[ \lambda \left[ \frac{d}{dr} - \frac{\lambda-1}{r} \right] + 1/\beta \right] \left[ r^{\lambda-1} e^{-r/\beta\nu} L_{k+1}^{2\lambda-1}(2r/\beta\nu) \right] \\ = - (k+\lambda+1-\nu)/\beta\nu r^{\lambda-1} e^{-r/\beta\nu} L_{k+1}^{2\lambda-1}(2r/\beta\nu) \\ - 2/(\beta\nu)^2 r^\lambda e^{-r/\beta\nu} L_k^{2\lambda+1}(2r/\beta\nu). \quad (2.3.30)$$

## CHAPTER 3 : THE SCHRODINGER-COULOMB GREEN FUNCTION

### 3.0 REDUCTION TO THE RADIAL EQUATION

The nonrelativistic hydrogenic Green function  $G(\mathbf{r}_1, \mathbf{r}_2; E)$  corresponding to the energy variable  $E$  is defined to be the solution of

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 - \frac{\hbar^2}{amr_1} - E \right] G(\mathbf{r}_1, \mathbf{r}_2; E) = \delta(\mathbf{r}_1 - \mathbf{r}_2) \quad (3.0.1)$$

subject to the boundary conditions that  $|G| \in L^2(\mathbb{R}^6)$ . In fact we will be solving (3.0.1) as a function of  $\mathbf{r}_1$  and thus require the less stringent condition that  $|G(\mathbf{r}_2)| \in L^2(\mathbb{R}^3)$  with  $G(\mathbf{r}_1, \mathbf{r}_2; E) = G(\mathbf{r}_2, \mathbf{r}_1; E)$ .

Due to the spherical symmetry of the the Schrodinger-Coulomb hamiltonian we are able to expand  $G$  in terms of spherical harmonics in the following manner<sup>4</sup>:

$$G(\mathbf{r}_1, \mathbf{r}_2; E) = \sum_{\ell m} g_{\ell}(r_1, r_2; E) Y_{\ell m}(\theta_1, \phi_1) Y_{\ell m}^*(\theta_2, \phi_2) \quad (3.0.2)$$

Noting also that

$$\delta(\mathbf{r}_1 - \mathbf{r}_2) = \frac{\delta(r_1 - r_2)}{r_1 r_2} \sum_{\ell m} Y_{\ell m}(\theta_1, \phi_1) Y_{\ell m}^*(\theta_2, \phi_2) \quad (3.0.3)$$

leads us to the defining equation for the radial part of the Schrodinger-Coulomb Green function,

$$\left[ \frac{1}{r_1^2} \frac{d}{dr_1} \left[ r_1^2 \frac{d}{dr_1} \right] - \frac{\ell(\ell+1)}{r_1^2} + \frac{2}{ar_1} - \frac{1}{\nu^2 a^2} \right] g_\ell(r_1, r_2; \nu) = - \frac{2m}{\hbar^2} \frac{\delta(r_1 - r_2)}{r_1 r_2} \quad (3.0.4)$$

where, as before  $\nu^2 a^2 = -\hbar^2/2mE$ . The boundary conditions we impose on  $g_\ell$  are:

$$\lim_{r_1 \rightarrow 0} r_1 g_\ell(r_1, r_2) = 0, \quad r_1 g_\ell \in L^2(\mathbb{R}). \quad (3.0.5)$$

As in our solution of the defining equations for the radial wavefunctions in the previous chapter, we find it convenient here to solve a slightly more general equation than the one given above. The advantage of doing this is that will become apparent when we come to discuss the Dirac-Coulomb Green function in the following chapter.

### 3.1 SOLUTION OF THE GENERALIZED RADIAL EQUATION

In this section we prove the following theorem

**THEOREM 2 :**

The solution of

$$\left[ \frac{d^2}{dr_1^2} + \frac{2}{r_1} \frac{d}{dr_1} - \frac{\lambda(\lambda+1)}{r_1^2} + \frac{2}{\beta r_1} - \frac{1}{\beta^2 \nu^2} \right] g(r_1, r_2) = - \frac{\delta(r_1 - r_2)}{r_1 r_2} \quad (3.1.1)$$

subject to the boundary conditions that

$$\lim_{r_1 \rightarrow 0} r_1 g(r_1, r_2) = 0 \quad ; \quad r_1 g(r_2) \in L^2(\mathbb{R}). \quad (3.1.2)$$

and where  $\lambda$ ,  $\beta$ , and  $\nu$  are positive real numbers, is

$$g(r_1, r_2) = \left[ \frac{2}{\beta\nu} \right]^{2\lambda+1} (r_1 r_2)^\lambda e^{-(r_1+r_2)/\beta\nu} \times \\ \times \sum_{k=0}^{\infty} \frac{k!}{\Gamma(2\lambda+2+k)(\lambda+1+k-\nu)} L_k^{2\lambda+1} \left[ \frac{2r_1}{\beta\nu} \right] L_k^{2\lambda+1} \left[ \frac{2r_2}{\beta\nu} \right] \quad (3.1.3)$$

*PROOF:* We proceed in a similar manner to the proof of THEOREM 1. the function

$$f(r_1, r_2) = (r_1 r_2)^{\lambda+1} g(r_1, r_2) \quad (3.1.4)$$

satisfies

$$\left[ r_1 \frac{d^2}{dr_1^2} - 2\lambda \frac{d}{dr_1} + \frac{2}{\beta} - \frac{r}{\beta^2 \nu^2} \right] f(r_1, r_2) = -r_1 (r_1 r_2)^\lambda \delta(r_1 - r_2) \quad (3.1.5)$$

The double Laplace transform<sup>37</sup> of  $f$ ,  $\mathcal{L}^2[f] \equiv F$  is

$$F(p_1, p_2) = \int_0^\infty \int_0^\infty e^{-p_1 r_1 - p_2 r_2} f(r_1, r_2) dr_1 dr_2 \quad (3.1.6)$$

and satisfies the transformed equation

$$\left[ (p_1^2 - 1/\beta^2 \nu^2) \frac{d}{dp_1} + 2p_1(\lambda+1) - 2/\beta \right] F(p_1, p_2) = \frac{\Gamma(2\lambda+2)}{(p_1+p_2)^{2\lambda+2}} \quad (3.1.7)$$

where we have used the fact that  $f(0, r_2) = 0$ . Now, letting

$$E(p_1, p_2) = \frac{(p_1+p_2)^{2\lambda+2}}{\Gamma(2\lambda+2)} F(p_1, p_2) \quad (3.1.8)$$

so that

$$\left[ (p_1^2 - 1/\beta^2\nu^2) \frac{d}{dp_1} + \frac{(2\lambda+2)}{(p_1+p_2)} (p_1 p_2 + 1/\beta^2\nu^2) - \frac{2}{\beta} \right] E(p_1, p_2) = 1, \quad (3.1.9)$$

and then making the change of variables

$$p_1 \mapsto z = -\beta\nu (p_1 - 1/\beta\nu)(p_2 - 1/\beta\nu)/2(p_1+p_2) \quad (3.1.10)$$

gives finally

$$\left[ z(1-z) \frac{d}{dz} + (\lambda+1)(1-2z) - \nu \right] E(z) = \beta\nu/2 \quad (3.1.11)$$

The solution to this last equation is easily found as a series in  $z$ , provided that  $\nu-\lambda-1$  is not an integer (which would not be true if we were considering the 'reduced' Schrodinger-Coulomb Green function). We find a particular solution to (3.1.11)

$$E_p(z) = \beta\nu {}_2F_1(2\lambda+2, 1; \lambda+2-\nu; z), \quad (3.1.12)$$

and a solution of the corresponding homogeneous equation

$$E_h(z) = N z^{\nu-\lambda-1} (z-1)^{-\nu-\lambda-1}, \quad (3.1.13)$$

where  $N$  is an arbitrary constant. Invoking a well known transformation of the hypergeometric function<sup>38</sup> we arrive at the general solution to (3.1.11) :

$$E(z) = \beta\nu (1-z)^{-2\lambda-2} {}_2F_1(2\lambda+2, \lambda+1-\nu; \lambda+2-\nu; \frac{z}{z-1}) / 2(\lambda-\nu+1) + N z^{\nu-\lambda-1} (z-1)^{-\nu-\lambda-1} \quad (3.1.14)$$

The double Laplace transform of  $f$  is therefore given by

$$F(p_1, p_2) = (2/\beta\nu)^{2\lambda+1} \frac{\Gamma(2\lambda+2)}{(\lambda-\nu+1)} [(p_1+1/\beta\nu)(p_2+1/\beta\nu)]^{-2\lambda-2} \times \\ \times {}_2F_1(2\lambda+2, \lambda+1-\nu; \lambda+2-\nu; \left[\frac{p_1-1/\beta\nu}{p_1+1/\beta\nu}\right] \left[\frac{p_2-1/\beta\nu}{p_2+1/\beta\nu}\right]) \\ + N [(p_1-1/\beta\nu)(p_2-1/\beta\nu)]^{\nu-\lambda-1} [(p_1+1/\beta\nu)(p_2+1/\beta\nu)]^{-\nu-\lambda-1} \quad (3.1.15)$$

Now, in terms of  $p_1$ ,  $F$  has a singularity of largest real part at  $p_1=1/\beta\nu$  if  $N \neq 0$ . As a consequence of a theorem on the asymptotic forms of functions and their Laplace transforms<sup>31</sup> we can infer that

$$g(r_1, r_2) \approx N r_1^{\lambda-\nu} e^{r_1/\beta\nu} \quad \text{as } r_1 \rightarrow \infty$$

which is at variance with the boundary conditions we have imposed. If  $\nu > \lambda+1$  there is, of course, no singularity at this point, but since we are looking for a solution valid for all real  $\nu$  and continuous in  $\nu$  we ignore that possibility. We deduce then, that  $N=0$ . Hence

$$F(p_1, p_2) = (2/\beta\nu)^{2\lambda+1} [(p_1+1/\beta\nu)(p_2+1/\beta\nu)]^{-2\lambda-2} \times \\ \times \sum_{k=0}^{\infty} \frac{\Gamma(2\lambda+2+k)}{(\lambda+1+k-\nu)k!} \left[\frac{p_1-1/\beta\nu}{p_1+1/\beta\nu}\right]^k \left[\frac{p_2-1/\beta\nu}{p_2+1/\beta\nu}\right]^k \quad (3.1.16)$$

The inverse double Laplace transform of  $F$  is easily obtained, since  $F$

itself is an infinite sum of products of single Laplace transforms<sup>37</sup>. Implicit in the proof of Theorem 1 was the fact that the Laplace transform of the Laguerre polynomial,

$$\begin{aligned} \mathcal{L} [r^\alpha L_n^\alpha(r)](p) &\equiv \int_0^\infty e^{-pr} r^\alpha L_n^\alpha(r) dr \\ &= \frac{\Gamma(\alpha+n+1) (p-1)^n}{n! p^{\alpha+n+1}} \quad \Re(\alpha) > -1, \Re(p) > 0 \end{aligned} \quad (3.1.17)$$

and thus

$$\mathcal{L} [e^{-r\sigma} r^\alpha L_n^\alpha(2r\sigma)](p) = \frac{\Gamma(\alpha+n+1) (p-\sigma)^n}{n! (p+\sigma)^{n+\alpha+1}} \quad \Re(\alpha) > -1, \Re(p) > -\sigma \quad (3.1.18)$$

We can now easily perform the inverse double Laplace transformation to get

$$\begin{aligned} f(r_1, r_2) &= (2/\beta\nu)^{2\lambda+1} (r_1 r_2)^{2\lambda+1} e^{-(r_1+r_2)/\beta\nu} \times \\ &\quad \sum_{k=0}^{\infty} \frac{k!}{\Gamma(2\lambda+2+k)(\lambda+1+k-\nu)} L_k^{2\lambda+1} \left[ \frac{2r_1}{\beta\nu} \right] L_k^{2\lambda+1} \left[ \frac{2r_2}{\beta\nu} \right] \end{aligned} \quad (3.1.19)$$

from which the theorem follows immediately. *QED.*

It is useful to note the points at which the boundary conditions have been used: (i) in the derivation of the transformed equation (3.1.7); (ii) in the deduction that the homogeneous part of the solution to (3.1.11) is unacceptable. The expansion of  $g$  in terms of Laguerre polynomials can be transformed quite generally into several other forms; rather than do that here we will consider the different forms of the Schrodinger- and

Dirac-Coulomb Green functions separately in the remainder of this chapter and in the following chapter. This treatment of the Laplace-transformed defining equation for the radial Green function, especially the use of the transformation (3.1.10) was independently discovered by Hill and Huxtable<sup>13</sup>, Talukdar et al.<sup>14</sup> and by myself. The derivation of the inverse Laplace transform is, it appears, new.

Before moving on to the analysis of the Schrodinger Coulomb Green function I will take this opportunity to present a representation of the Dirac delta function which will be of use later on. We have exhibited explicitly the solution to (3.1.1); furthermore, we can easily calculate the effect of the differential operator on this solution using results obtained in the previous chapter. Thus, substituting (3.1.3) directly into (3.1.1) leads to the following interesting formula:

$$\alpha^{2\lambda+2} (xy)^\lambda e^{-\alpha(x+y)/2} \sum_{k=0}^{\infty} \frac{k!}{\Gamma(2\lambda+2+k)} L_k^{2\lambda+1}(\alpha x) L_k^{2\lambda+1}(\alpha y) = \delta(x-y)/\sqrt{xy} \quad (3.1.20)$$

This can be thought of as either a representation of the delta function, or as an expression for the infinite sum of Laguerre polynomials or as a direct proof of the completeness of the Sturmian wavefunctions.

### 3.2 FORMS OF THE SCHRODINGER-COULOMB GREEN FUNCTION.

We can now immediately write down the so-called Sturmian form of the radial Schrodinger-Coulomb Green function<sup>10</sup>,



[A]

$$g_\ell(r_1, r_2; \nu) = (2m/\hbar^2) (2/a\nu)^{2\ell+1} (r_1 r_2)^\ell e^{-(r_1+r_2)/a\nu} \times \sum_{k=0}^{\infty} \frac{k!}{(2\ell+1+k)!(\ell+1+k-\nu)} L_k^{2\ell+1}\left[\frac{2r_1}{a\nu}\right] L_k^{2\ell+1}\left[\frac{2r_2}{a\nu}\right] \quad (3.2.1)$$

Notice the poles at  $n \equiv \nu = \ell+1+k$  corresponding to the energy eigenvalues  $E_n = -(\alpha Z)^2 m c^2 / 2n^2$ , with  $\ell = 0, \dots, n-1$ . Thus we have obtained, *en passant*, the discrete part of the hydrogenic spectrum. It is often remarked that the Schrodinger-Coulomb Green function can be expressed as a sum over the discrete spectrum alone. We see it as a consequence of our solution of the defining differential equation.

We refer to the above as form [A] of  $g_\ell$ . We now proceed to derive several additional forms. We begin with the following representation of the modified Bessel function<sup>39</sup>,

$$\begin{aligned} \left[\frac{2r_1 2r_2}{a\nu a\nu} t\right]^{-\ell-1/2} (1-t)^{\nu-1} \exp\left[-\frac{t}{1-t} \frac{2}{a\nu} (r_1+r_2)\right] I_{2\ell+1}\left[\frac{4\sqrt{r_1 r_2 t}}{a\nu(1-t)}\right] = \\ = \sum_{k=0}^{\infty} \frac{k!}{(2\ell+1+k)!} t^k L_k^{2\ell+1}\left[\frac{2r_1}{a\nu}\right] L_k^{2\ell+1}\left[\frac{2r_2}{a\nu}\right] \end{aligned} \quad (3.2.2)$$

together with

$$\int_0^1 t^{\ell+k-\nu} dt = (\ell+k+1-\nu)^{-1} \quad (3.2.3)$$

to arrive at our first variant on [A]:

[B]

$$g_\ell(r_1, r_2; \nu) = (2m/\hbar^2) \frac{1}{\sqrt{r_1 r_2}} \int_0^1 t^{-\nu-\frac{1}{2}} (1-t)^{-1} \exp\left[-\frac{(r_1+r_2)(1+t)}{a\nu(1-t)}\right] \times \\ \times I_{2\ell+1}\left[\frac{4\sqrt{r_1 r_2} t}{a\nu(1-t)}\right] dt. \quad (3.2.4)$$

Now we make a change of variables  $t \mapsto s = 1-t$  and find

[C]

$$g_\ell(r_1, r_2; \nu) = (2m/\hbar^2) \frac{1}{\sqrt{r_1 r_2}} e^{(r_1+r_2)/a\nu} \times \\ \int_0^1 (1-s)^{-\nu-\frac{1}{2}} s^{-1} \exp\left[-\frac{2(r_1+r_2)}{a\nu s}\right] I_{2\ell+1}\left[\frac{4\sqrt{r_1 r_2}(1-s)}{a\nu s}\right] ds. \quad (3.2.5)$$

As a final change of variable of integration we let  $s \mapsto \rho = \cosh^{-1}(2/s-1)$  to arrive at a form of  $g_\ell$  which has been frequently used by other authors:<sup>6</sup>

[D]

$$g_\ell(r_1, r_2; \nu) = (2m/\hbar^2) \frac{1}{\sqrt{r_1 r_2}} \int_0^\infty (\coth \frac{\rho}{2})^{2\nu} \exp\left[-\frac{(r_1+r_2)}{a\nu} \cosh \rho\right] \times \\ \times I_{2\ell+1}\left[\frac{2\sqrt{r_1 r_2}}{a\nu} \sinh \rho\right] d\rho. \quad (3.2.6)$$

We can now write down the 'standard' representation of the radial Schrodinger-Coulomb Green function in terms of regular and irregular Whittaker functions,  $M$  and  $W$  by noting that<sup>40</sup>

$$W_{\nu, \mu/2}(a_1 t) M_{\nu, \mu/2}(a_2 t) = \frac{t\sqrt{a_1 a_2} \Gamma(\mu+1)}{\Gamma(1/2+\mu/2-\nu)} \int_0^\infty (\coth \frac{\rho}{2})^{2\nu} \times \\ \exp\left[-\frac{(a_1+a_2)}{2} t \cosh \rho\right] I_\mu(t\sqrt{a_1 a_2} \sinh \rho) d\rho \quad (3.2.7)$$

(for  $\Re(1/2+\mu/2-\nu) > 0$ ,  $\Re(t) > 0$ ,  $a_1 > a_2$ ) from which follows<sup>6</sup>

[E]

$$g_\ell(r_1, r_2; \nu) = \frac{m a \nu}{\hbar^2} \frac{\Gamma(\ell+1-\nu)}{(2\ell+1)!} \frac{1}{r_1 r_2} M_{\nu, \ell+\frac{1}{2}} \left[ \frac{2r}{a\nu} < \right] W_{\nu, \ell+\frac{1}{2}} \left[ \frac{2r}{a\nu} > \right], \quad (3.2.8)$$

where  $r_< = \min\{r_1, r_2\}$  and  $r_> = \max\{r_1, r_2\}$ .

Further representations will be found to be useful. Returning to equation (3.2.1) and noting that<sup>39</sup>

$$e^{-z} z^{\alpha/2} L_n^\alpha(z) = \frac{1}{n!} \int_0^\infty e^{-s} s^{n+\alpha/2} J_\alpha(2\sqrt{sz}) ds \quad (3.2.9)$$

where  $n+\Re(\alpha) > -1$  and  $J_\alpha$  is a Bessel function we find a double integral formula for  $g_\ell$ :

[F]

$$g_\ell(r_1, r_2; \nu) = (2m/\hbar^2) \frac{e^{(r_1+r_2)/a\nu}}{\sqrt{r_1 r_2}} \int_0^\infty \int_0^\infty e^{-s_1-s_2} J_{2\ell+1} \left[ 2\sqrt{\frac{2r_1 s_1}{a\nu}} \right] \times \\ \times J_{2\ell+1} \left[ 2\sqrt{\frac{2r_2 s_2}{a\nu}} \right] \sum_{k=0}^\infty \frac{(s_1 s_2)^{k+\ell+\frac{1}{2}}}{(2\ell+1+k)! k! (\ell+1+k-\nu)} ds_1 ds_2. \quad (3.2.10)$$

The sum in the last equation can be expressed as an integral over a modified Bessel function using equation (3.2.3),

$$\sum_{k=0}^\infty \frac{(s_1 s_2)^{k+\ell+\frac{1}{2}}}{(2\ell+1+k)! k! (\ell+1+k-\nu)} = \int_0^\infty t^{-\nu-\frac{1}{2}} I_{2\ell+1}(2\sqrt{s_1 s_2} t) dt \quad (3.2.11)$$

and this leads us to our final form for the radial Schrodinger-Coulomb Green function:

[G]

$$g_\ell(r_1, r_2; \nu) = (2m/\hbar^2) \frac{e^{(r_1+r_2)/a\nu}}{\sqrt{r_1 r_2}} \int_0^\infty \int_0^\infty e^{-s_1-s_2} J_{2\ell+1} \left[ 2\sqrt{\frac{2r_1 s_1}{a\nu}} \right] \times \\ \times J_{2\ell+1} \left[ 2\sqrt{\frac{2r_2 s_2}{a\nu}} \right] \int_0^\infty t^{-\nu-\frac{1}{2}} I_{2\ell+1}(2\sqrt{s_1 s_2 t}) dt ds_1 ds_2. \quad (3.2.12)$$

It is interesting to note that by performing the integrals over  $s_1$  and  $s_2$  in (3.2.12) we arrive at [B] equation (3.2.4).

We now take a step backwards. From (3.0.2)

$$G(r_1, r_2; E) = \sum_{\ell m} g_\ell(r_1, r_2; \nu) Y_{\ell m}(\theta_1, \phi_1) Y_{\ell m}^*(\theta_2, \phi_2) \\ = \sum_{\ell} g_\ell(r_1, r_2; \nu) (2\ell+1) P_\ell(\hat{r}_1 \cdot \hat{r}_2) \quad (3.2.13)$$

where  $P_\ell$  is a Legendre polynomial of degree  $\ell$ . In view of (3.2.5) we can write

$$G(r_1, r_2; E) = (2m/\hbar^2) \frac{1}{\sqrt{r_1 r_2}} \int_0^\infty (\cosh \frac{\rho}{2})^{2\nu} \exp \left[ -\frac{(r_1+r_2)}{a\nu} \cosh \rho \right] \\ \times \sum_{\ell} (2\ell+1) P_\ell(\hat{r}_1 \cdot \hat{r}_2) I_{2\ell+1} \left[ \frac{2\sqrt{r_1 r_2}}{a\nu} \sinh \rho \right] d\rho,$$

and, since

$$\rho/2 I_0(\rho\sqrt{(1+\tau)/2}) = \sum_{\ell} (2\ell+1) P_\ell(\tau) I_{2\ell+1}(\rho), \quad (3.2.14)$$

[H]

$$G(\hat{r}_1, \hat{r}_2; E) = (2m/\hbar^2 a\nu) \int_0^\infty (\coth \frac{\rho}{2})^{2\nu} \sinh \rho \exp\left[-\frac{(r_1+r_2)}{a\nu} \cosh \rho\right] \\ \times I_0\left[\frac{\sinh \rho}{a\nu} \sqrt{2r_1 r_2 (1+\hat{r}_1 \cdot \hat{r}_2)}\right] d\rho \quad (3.2.15)$$

This form was first presented by Hostler<sup>6</sup>. We can of course resort to a variable we have used previously:  $\rho \leftrightarrow t$  where  $\cosh \rho = (1+t)/(1-t)$ . Then (3.2.15) becomes

[I]

$$G(\hat{r}_1, \hat{r}_2; E) = (2m/\hbar^2 a\nu) \int_0^\infty \frac{2t^{-\nu}}{(1-t)^2} \exp\left[-\frac{(r_1+r_2)}{a\nu} \frac{1+t}{1-t}\right] \\ \times I_0\left[\frac{2[2tr_1 r_2 (1+\hat{r}_1 \cdot \hat{r}_2)]^{\frac{1}{2}}}{a\nu(1-t)}\right] dt \quad (3.2.16)$$

We are now in a position to find a 'Sturmian' expansion of the Schrodinger-Coulomb Green function in parabolic coordinates. Recalling from Chapter 2 the definition of this coordinate system it is not difficult to show that

$$2r_1 r_2 (1+\hat{r}_1 \cdot \hat{r}_2) = \xi_1 \xi_2 + \eta_1 \eta_2 + 2\sqrt{\xi_1 \xi_2 \eta_1 \eta_2} \cos(\varphi_2 - \varphi_1) \quad (3.2.17)$$

We also note (Lebedev ref.39) that

$$I_0(\sqrt{a^2+b^2+2ab\cos\theta}) = \sum_{m=-\infty}^{+\infty} (-1)^m e^{im\theta} I_m(a) I_m(b) \quad (3.2.18)$$

Thus, from (3.2.16) we can write

$$G(r_1, r_2; E) = \sum_{m=-\infty}^{+\infty} (-1)^m e^{im(\varphi_1 - \varphi_2)} g_m(\xi_1, \eta_1; \xi_2, \eta_2; \nu) \quad (3.2.19)$$

where<sup>12</sup>

[J]

$$g_m(\xi_1, \eta_1; \xi_2, \eta_2; \nu) = (4m/\hbar^2 a\nu) \int_0^\infty \frac{t^{-\nu}}{(1-t)^2} \exp \left[ \left( \frac{(\xi_1 + \eta_1 + \xi_2 + \eta_2)}{2a\nu} \right) \left( \frac{1+t}{1-t} \right) \right] \\ \times I_m \left[ \frac{2\sqrt{t\xi_1\xi_2}}{a\nu(1-t)} \right] I_m \left[ \frac{2\sqrt{t\eta_1\eta_2}}{a\nu(1-t)} \right] dt \quad (3.2.20)$$

Now, as in (3.2.2) we can write

$$I_m \left[ \frac{2\sqrt{t\xi_1\xi_2}}{a\nu(1-t)} \right] = (1-t) \exp \left[ \frac{t(\xi_1 + \xi_2)}{a\nu(1-t)} \right] \left[ \frac{t\xi_1\xi_2}{a^2\nu^2} \right]^{|m|/2} \sum_{k=0}^{\infty} \frac{k!}{(k+|m|)!} t^k \\ \times L_k^{|m|}(\xi_1/a\nu) L_k^{|m|}(\xi_2/a\nu) \quad (3.2.21)$$

since  $I_m = I_{-m}$ . Thus we arrive at the following form of the Green function in parabolic coordinates:

[K]

$$g_m(\xi_1, \eta_1; \xi_2, \eta_2; \nu) = \frac{(4m/\hbar^2)}{(a\nu)^{2|m|+1}} (\xi_1 \xi_2 \eta_1 \eta_2)^{|m|/2} \exp \left[ -\frac{(\xi_1 + \xi_2 + \eta_1 + \eta_2)}{2a\nu} \right] \\ \times \sum_{i,j} \frac{i!j!}{(i+|m|)!} \frac{(i+j+|m|+1-\nu)^{-1}}{(j+|m|)!} L_i^{|m|} \left[ \frac{\xi_1}{a\nu} \right] L_j^{|m|} \left[ \frac{\eta_1}{a\nu} \right] L_i^{|m|} \left[ \frac{\xi_2}{a\nu} \right] L_j^{|m|} \left[ \frac{\eta_2}{a\nu} \right] \quad (3.2.22)$$

Form [J] of the Schrodinger-Coulomb Green function has been found to be of interest in several studies of the phase space formulation of quantum mechanics. I can find no reference to the Sturmian form [K] in literature.

## 3.3 : AN INTEGRAL EQUATION

Lebedev<sup>39</sup> shows that

$$e^{-\rho/2} \rho^{\alpha/2} L_n^\alpha(\rho) = (-1)^{n/2} \int_0^\infty J_\alpha(\sqrt{\rho\tau}) e^{-\tau/2} \tau^{\alpha/2} L_n^\alpha(\tau) d\tau \quad (3.3.1)$$

for  $\alpha > -1$ ,  $n=0,1,\dots$  Substituting this into the Sturmian form of  $g_\ell$  we quickly find that

$$\begin{aligned} \sqrt{r_1 r_2} g_\ell(r_1, r_2; \nu) &= (1/a\nu)^2 \int_0^\infty J_{2\ell+1}\left[\frac{2\sqrt{r_1 s_1}}{a\nu}\right] J_{2\ell+1}\left[\frac{2\sqrt{r_2 s_2}}{a\nu}\right] \\ &\quad \times \sqrt{s_1 s_2} g_\ell(s_1, s_2; \nu) ds_1 ds_2 . \end{aligned} \quad (3.3.2)$$

This property has some interesting consequences for the double Laplace transforms we shall be considering in Chapter 5.

## CHAPTER 4 : THE DIRAC-COULOMB GREEN FUNCTION

### 4.1 : REDUCTION TO THE RADIAL EQUATION

The relativistic Coulomb Green function  $G(\vec{r}_1, \vec{r}_2; E)$  corresponding to the energy variable  $E$  is the  $4 \times 4$  matrix function satisfying

$$\left[ (\vec{\alpha} \cdot \vec{r}_1) \left[ -\frac{i\hbar c}{r_1} \frac{d}{dr_1} r_1 + \frac{ic}{r_1} \beta \vec{K} \right] + \beta mc^2 - \frac{\alpha Z \hbar c}{r_1} - E \right] G(\vec{r}_1, \vec{r}_2; E) = \delta(\vec{r}_1 - \vec{r}_2) I_4 \quad (4.1.1)$$

subject to suitable boundary conditions. Taking our lead from the treatment we made of the nonrelativistic Green function we expand  $G$  in the spinorial equivalent of spherical harmonics, that is in terms of the spinor spherical harmonics we introduced in Chapter 2. Thus we try a solution of the form<sup>16</sup>

$$G(\vec{r}_1, \vec{r}_2; E) = \sum_{\kappa \mu} \begin{bmatrix} g_{\kappa}^{11}(r_1, r_2) \chi_{\kappa}^{\mu}(\vec{r}_1) \chi_{\kappa}^{\mu \dagger}(\vec{r}_2) & -ig_{\kappa}^{12}(r_1, r_2) \chi_{\kappa}^{\mu}(\vec{r}_1) \chi_{-\kappa}^{\mu \dagger}(\vec{r}_2) \\ ig_{\kappa}^{21}(r_1, r_2) \chi_{-\kappa}^{\mu}(\vec{r}_1) \chi_{\kappa}^{\mu \dagger}(\vec{r}_2) & g_{\kappa}^{22}(r_1, r_2) \chi_{-\kappa}^{\mu}(\vec{r}_1) \chi_{-\kappa}^{\mu \dagger}(\vec{r}_2) \end{bmatrix} \quad (4.1.2)$$

Noting that<sup>36</sup>

$$\vec{\sigma} \cdot \vec{r} \chi_{\kappa}^{\mu} = -\chi_{-\kappa}^{\mu} \quad (4.1.3)$$

and,



$$(\vec{\sigma} \cdot \vec{L} + \hbar) \chi_{\kappa}^{\mu} = -\hbar\kappa \chi_{\kappa}^{\mu} \quad (4.1.4)$$

equation (4.1.1) becomes

$$\sum_{\kappa\mu} \begin{bmatrix} A_{11}^{\kappa\mu} & A_{12}^{\kappa\mu} \\ A_{21}^{\kappa\mu} & A_{22}^{\kappa\mu} \end{bmatrix} = \delta(\hat{r}_1 - \hat{r}_2) I_4 / \hbar c \quad (4.1.5)$$

where

$$A_{11}^{\kappa\mu} = \left[ (\epsilon_0 - \epsilon - \alpha Z/r_1) g_{\kappa}^{11} + \left[ -\frac{1}{r_1} \frac{d}{dr_1} r_1 + \frac{\kappa}{r_1} \right] g_{\kappa}^{21} \right] \chi_{\kappa}^{\mu}(\hat{r}_1) \chi_{\kappa}^{\mu\dagger}(\hat{r}_2) \quad (4.1.6a)$$

$$A_{12}^{\kappa\mu} = i \left[ -(\epsilon_0 - \epsilon - \alpha Z/r_1) g_{\kappa}^{12} + \left[ \frac{1}{r_1} \frac{d}{dr_1} r_1 - \frac{\kappa}{r_1} \right] g_{\kappa}^{22} \right] \chi_{\kappa}^{\mu}(\hat{r}_1) \chi_{-\kappa}^{\mu\dagger}(\hat{r}_2) \quad (4.1.6b)$$

$$A_{21}^{\kappa\mu} = i \left[ \left[ \frac{1}{r_1} \frac{d}{dr_1} r_1 + \frac{\kappa}{r_1} \right] g_{\kappa}^{11} - (\epsilon_0 + \epsilon + \alpha Z/r_1) g_{\kappa}^{21} \right] \chi_{-\kappa}^{\mu}(\hat{r}_1) \chi_{\kappa}^{\mu\dagger}(\hat{r}_2) \quad (4.1.6c)$$

$$A_{22}^{\kappa\mu} = \left[ \left[ \frac{1}{r_1} \frac{d}{dr_1} r_1 + \frac{\kappa}{r_1} \right] g_{\kappa}^{12} - (\epsilon_0 + \epsilon + \alpha Z/r_1) g_{\kappa}^{22} \right] \chi_{-\kappa}^{\mu}(\hat{r}_1) \chi_{-\kappa}^{\mu\dagger}(\hat{r}_2) \quad (4.1.6d)$$

Here we have suppressed the  $r$ -dependence of the  $g$ 's and we have written

$$\epsilon_0 = mc^2/\hbar c, \quad \epsilon = E/\hbar c \quad (4.1.7)$$

Now we use the fact that

$$\delta(\hat{r}_1 - \hat{r}_2) I_2 = \delta(r_1 - r_2)/(r_1 r_2) \sum_{\kappa\mu} \chi_{\kappa}^{\mu}(\theta_1, \phi_1) \chi_{\kappa}^{\mu\dagger}(\theta_2, \phi_2) \quad (4.1.8)$$

to write

$$\delta(\hat{r}_1 - \hat{r}_2) I_4 = \delta(r_1 - r_2) / (r_1 r_2) \sum_{\kappa \mu} \begin{bmatrix} \chi_{\kappa}^{\mu}(\hat{r}_1) \chi_{\kappa}^{\mu \dagger}(\hat{r}_2) & 0 \\ 0 & \chi_{-\kappa}^{\mu}(\hat{r}_1) \chi_{-\kappa}^{\mu \dagger}(\hat{r}_2) \end{bmatrix} \quad (4.1.9)$$

Now, employing the orthonormality properties of the spinor spherical harmonics we see that (4.1.5) and (4.1.9) lead to

$$\begin{bmatrix} [\epsilon_0 - \epsilon - \alpha Z / r_1] & \left[ -\frac{1}{r_1} \frac{d}{dr_1} r_1 + \frac{\kappa}{r_1} \right] \\ \left[ \frac{1}{r_1} \frac{d}{dr_1} r_1 + \frac{\kappa}{r_1} \right] & [-\epsilon_0 - \epsilon - \alpha Z / r_1] \end{bmatrix} \begin{bmatrix} g_{\kappa}^{11} & g_{\kappa}^{12} \\ g_{\kappa}^{21} & g_{\kappa}^{22} \end{bmatrix} = \frac{\delta(r_1 - r_2)}{r_1 r_2} I_2 / \hbar c. \quad (4.1.10)$$

These are the radial equations we must solve. In the next section we perform a linear transformation which will reduce (4.1.10) to a form which will allow us to use Theorem 2 which was proved in the last Chapter. From now on we will dispense with the subscript  $\kappa$  on the  $g$ 's it being understood that  $\kappa$  is now a fixed parameter.

## 4.2 : TRANSFORMATION OF THE RADIAL EQUATIONS

Let

$$\begin{bmatrix} f^{11} & f^{12} \\ f^{21} & f^{22} \end{bmatrix} = \underline{X} \begin{bmatrix} g^{11} & g^{12} \\ g^{21} & g^{22} \end{bmatrix} \quad (4.2.1)$$

where

$$\underline{X} = \begin{bmatrix} 1 & \kappa \\ \kappa & 1 \end{bmatrix} \quad (4.2.2)$$

and  $\kappa$  is to be determined. Then, since

$$\underline{X}^{-1} = (1-\kappa^2)^{-1} \begin{bmatrix} 1 & -\kappa \\ -\kappa & 1 \end{bmatrix} \quad (4.2.3)$$

the radial equations (4.1.10) become

$$\begin{bmatrix} \left[ \epsilon_0 - \epsilon - \frac{(\alpha Z + \kappa \kappa - \kappa)}{r_1} + \kappa \frac{d}{dr_1} \right] & \left[ -\kappa \epsilon_0 + \kappa \epsilon + \frac{(\alpha Z \kappa + \kappa - 1)}{r_1} - \frac{d}{dr_1} \right] \\ \left[ \kappa \epsilon_0 + \kappa \epsilon + \frac{(\alpha Z \kappa + \kappa + 1)}{r_1} + \frac{d}{dr_1} \right] & \left[ -\epsilon_0 - \epsilon - \frac{(\alpha Z + \kappa \kappa + \kappa)}{r_1} - \kappa \frac{d}{dr_1} \right] \end{bmatrix} \times \\ \times \begin{bmatrix} f_{11} & f_{12} \\ f_{21} & f_{22} \end{bmatrix} = \frac{(1-\kappa^2)}{\hbar c} \frac{\delta(r_1 - r_2)}{r_1 r_2} I_2 \quad (4.2.4)$$

We continue to follow the method employed in the reduction of the radial equations for the Dirac-Coulomb problem by eliminating the derivatives from the diagonal terms. This is achieved by premultiplying equation (4.2.4) by  $\underline{X}^{-1}$  so that

$$\begin{bmatrix} \left[ (1-\kappa^2) \epsilon_0 - (1+\kappa^2) \epsilon - \frac{A}{r_1} \right] & \left[ 2\kappa \epsilon + \frac{B}{r_1} - (1-\kappa^2) \frac{d}{dr_1} \right] \\ \left[ 2\kappa \epsilon + \frac{B}{r_1} + (1-\kappa^2) \frac{d}{dr_1} \right] & \left[ (\kappa^2 - 1) \epsilon_0 - (1+\kappa^2) \epsilon - \frac{A}{r_1} \right] \end{bmatrix} \times \\ \times \begin{bmatrix} f_{11} & f_{12} \\ f_{21} & f_{22} \end{bmatrix} = \frac{(1-\kappa^2)^2}{\hbar c} \frac{\delta(r_1 - r_2)}{r_1 r_2} \underline{X}^{-1} \quad (4.2.5)$$

where

$$A = (1+\aleph^2)\alpha Z + 2\aleph\kappa, \quad B = 2\alpha Z\aleph + (1+\aleph^2)\kappa - (1-\aleph^2). \quad (4.2.6)$$

We now choose  $\aleph$  in such a way that  $A$  vanishes; that is we make the same choice for  $\aleph$  as before,  $\aleph = (-\kappa + \gamma)/\alpha Z$  with  $\gamma = \sqrt{\kappa^2 - \alpha^2 Z^2}$ . The radial equations simplify considerably to

$$\begin{aligned} & \begin{bmatrix} \left[ \frac{\gamma}{\kappa} \epsilon_0 - \epsilon \right] & \left[ \frac{\alpha Z \epsilon}{\kappa} + \frac{\gamma(\gamma-1)}{\kappa r_1} - \frac{\gamma}{\kappa} \frac{d}{dr_1} \right] \\ \left[ \frac{\alpha Z \epsilon}{\kappa} + \frac{\gamma(\gamma+1)}{\kappa r_1} + \frac{\gamma}{\kappa} \frac{d}{dr_1} \right] & \left[ -\frac{\gamma}{\kappa} \epsilon_0 - \epsilon \right] \end{bmatrix} \times \\ & \times \begin{bmatrix} f^{11} & f^{12} \\ f^{21} & f^{22} \end{bmatrix} = \gamma/(\kappa \hbar c) \frac{\delta(r_1 - r_2)}{r_1 r_2} (1 - \aleph^2) \underline{X}^{-1} \end{aligned} \quad (4.2.7)$$

or, on dividing by  $\gamma/\kappa$ ,

$$\begin{aligned} & \begin{bmatrix} \left[ \epsilon_0 - \kappa \epsilon / \gamma \right] & \left[ \frac{-\alpha Z \epsilon}{\gamma} + \frac{\gamma-1}{r} - \frac{d}{dr} \right] \\ \left[ \frac{-\alpha Z \epsilon}{\gamma} + \frac{\gamma+1}{r} + \frac{d}{dr} \right] & \left[ -\epsilon_0 - \kappa \epsilon / \gamma \right] \end{bmatrix} \begin{bmatrix} f^{11} & f^{12} \\ f^{21} & f^{22} \end{bmatrix} = \\ & = (1 - \aleph^2) / \hbar c \frac{\delta(r_1 - r_2)}{r_1 r_2} \underline{X}^{-1} \end{aligned} \quad (4.2.8)$$

The final step, which does not arise in the solution of the Dirac-Coulomb equation, is to diagonalize the right hand side of (4.2.8). Thus we define

$$\begin{bmatrix} h^{11} & h^{12} \\ h^{21} & h^{22} \end{bmatrix} = \begin{bmatrix} f^{11} & f^{12} \\ f^{21} & f^{22} \end{bmatrix} \times \underline{X} \quad (4.2.9)$$

so that, on post multiplying (4.2.8) by  $\underline{X}$ , we have

$$\begin{aligned}
 & \begin{bmatrix} \left[ \epsilon_0 - \epsilon\kappa/\gamma \right] & \left[ -\frac{\alpha Z\epsilon}{\gamma} + \frac{\gamma-1}{r_1} - \frac{d}{dr_1} \right] \\ \left[ -\frac{\alpha Z\epsilon}{\gamma} + \frac{\gamma+1}{r_1} + \frac{d}{dr_1} \right] & \left[ -\epsilon_0 - \epsilon\kappa/\gamma \right] \end{bmatrix} \begin{bmatrix} h^{11} & h^{12} \\ h^{21} & h^{22} \end{bmatrix} = \\
 & = (1-\kappa^2)/\hbar c \frac{\delta(r_1-r_2)}{r_1 r_2} I_2. \quad (4.2.10)
 \end{aligned}$$

The overall transformation is given by

$$\begin{bmatrix} h^{11} & h^{12} \\ h^{21} & h^{22} \end{bmatrix} = \underline{X} \begin{bmatrix} g^{11} & g^{12} \\ g^{21} & g^{22} \end{bmatrix} \underline{X}. \quad (4.2.11)$$

We can now consider the four equations embodied in (4.2.10) in two pairs, since there is no mixing of the columns of the  $h$ -matrix. Firstly,

$$\left[ \epsilon_0 - \epsilon\kappa/\gamma \right] h^{11} + \left[ -\frac{\alpha Z\epsilon}{\gamma} + \frac{\gamma-1}{r_1} - \frac{d}{dr_1} \right] h^{21} = \frac{(1-\kappa^2)}{\hbar c} \frac{\delta(r_1-r_2)}{r_1 r_2} \quad (4.2.12a)$$

$$\left[ -\frac{\alpha Z\epsilon}{\gamma} + \frac{\gamma+1}{r_1} + \frac{d}{dr_1} \right] h^{11} - \left[ \epsilon_0 + \epsilon\kappa/\gamma \right] h^{21} = 0 \quad (4.2.12b)$$

Substituting (4.2.12b) into (4.2.12a) gives

$$\begin{aligned}
 & \left[ \frac{d^2}{dr_1^2} + \frac{2}{r_1} \frac{d}{dr_1} - \frac{\gamma(\gamma+1)}{r_1^2} + \frac{2\alpha Z\epsilon}{r_1} + \epsilon_0^2 - \epsilon_0^2 \right] h^{11} \\
 & = (\epsilon_0 + \epsilon\kappa/\gamma) \frac{(1-\kappa^2)}{\hbar c} \frac{\delta(r_1-r_2)}{r_1 r_2} \quad (4.2.13a)
 \end{aligned}$$

and

$$h^{21} = \gamma/(\epsilon\kappa + \epsilon_0\gamma) \left[ -\frac{\alpha Z\epsilon}{\gamma} + \frac{\gamma+1}{r_1} + \frac{d}{dr_1} \right] h^{11} \quad (4.2.13b)$$

The second pair of equations are

$$\left[ \epsilon_0 - \epsilon\kappa/\gamma \right] h^{12} + \left[ -\frac{\alpha Z\epsilon}{\gamma} + \frac{\gamma-1}{r_1} - \frac{d}{dr_1} \right] h^{22} = 0 \quad (4.2.14a)$$

$$\left[ -\frac{\alpha Z\epsilon}{\gamma} + \frac{\gamma+1}{r_1} + \frac{d}{dr_1} \right] h^{12} - \left[ \epsilon_0 + \epsilon\kappa/\gamma \right] h^{22} = \frac{(1-K^2)}{\hbar c} \frac{\delta(r_1-r_2)}{r_1 r_2} \quad (4.2.14b)$$

On substitution,

$$\left[ \frac{d^2}{dr_1^2} + \frac{2}{r_1} \frac{d}{dr_1} - \frac{\gamma(\gamma-1)}{r_1^2} + \frac{2\alpha Z\epsilon}{r_1} + \epsilon^2 - \epsilon_0^2 \right] h^{22} = (\epsilon_0 - \epsilon\kappa/\gamma) \frac{(1-K^2)}{\hbar c} \frac{\delta(r_1-r_2)}{r_1 r_2} \quad (4.2.15a)$$

and

$$h^{12} = \gamma/(\epsilon\kappa - \epsilon_0\gamma) \left[ -\frac{\alpha Z\epsilon}{\gamma} + \frac{\gamma-1}{r_1} - \frac{d}{dr_1} \right] h^{22} \quad (4.2.15b)$$

It is clear from the from of equations (4.2.13a) and (4.2.15a) that  $h^{11}$  and  $h^{22}$  can be calculated using THEOREM 2 proven in Chapter 3 and used there to calculate the radial part of the Schrodinger-Coulomb Green function. We have found then, that relatively simple transformations can be found to reduce both the Dirac wavefunctions and Green functions to their nonrelativistic counterparts.

### 4.3 : FORMS OF THE RADIAL DIRAC-COULOMB GREEN FUNCTIONS.

The diagonal terms are clearly closely related. Given THEOREM 2

we see from (4.2.13a) and (4.2.15a) that

$$h^{11}(r_1, r_2) = (1 - \kappa^2)(\epsilon \kappa + \epsilon_0 \gamma) / (\hbar c \gamma) h(r_1, r_2; \gamma, \omega) \quad (4.3.1)$$

and

$$h^{22}(r_1, r_2) = (1 - \kappa^2)(\epsilon \kappa - \epsilon_0 \gamma) / (\hbar c \gamma) h(r_1, r_2; \gamma - 1, \omega) \quad (4.3.2)$$

where

$$h(r_1, r_2; \lambda, \omega) = (2\omega)^{2\lambda+1} (r_1 r_2)^\lambda e^{-(r_1+r_2)\omega} \times \sum_{k=0}^{\infty} \frac{k! (k+1+\lambda-\nu)^{-1}}{\Gamma(2\lambda+2+k)} L_k^{2\lambda+1}(2r_1\omega) L_k^{2\lambda+1}(2r_2\omega) \quad (4.3.3)$$

and  $\nu = \alpha Z \epsilon / \sqrt{\epsilon_0^2 - \epsilon^2}$  and  $\omega = \sqrt{\epsilon_0^2 - \epsilon^2}$ .

We may derive various other representations just as we did for the Schrodinger-Coulomb Green function. Hence, in exactly the same manner as was used in Chapter III we find

$$h(r_1, r_2; \lambda, \omega) = 1/\sqrt{r_1 r_2} e^{(r_1+r_2)\omega} \int_0^\infty \int_0^\infty e^{-s_1-s_2} J_{2\lambda+1}(2\sqrt{2\omega r_1 s_1}) \times J_{2\lambda+1}(2\sqrt{2\omega r_2 s_2}) \sum_{k=0}^{\infty} \frac{(s_1 s_2)^{k+\lambda+\frac{1}{2}}}{\Gamma(2\lambda+2+k) k! (\lambda+1+k-\nu)} ds_1 ds_2 \quad (4.3.4)$$

$$= 1/\sqrt{r_1 r_2} \int_0^1 t^{-\nu-\frac{1}{2}}(1-t) \exp(-\omega[r_1+r_2][1+t]/[1-t]) \times I_{2\lambda+1}(4\omega\sqrt{r_1 r_2} t/[1-t]) dt \quad (4.3.5)$$

$$\begin{aligned}
&= 1/\sqrt{r_1 r_2} e^{(r_1+r_2)\omega} \times \int_0^1 (1-s)^{\nu-\frac{1}{2}} s^{-1} \exp(-2\omega[r_1+r_2]/s) \\
&\quad \times I_{2\lambda+1}(4\omega\sqrt{r_1 r_2}[1-s]/s) ds \quad (4.3.6)
\end{aligned}$$

$$\begin{aligned}
&= 1/\sqrt{r_1 r_2} \int_0^\infty (\coth \frac{\sigma}{2})^{2\nu} \exp(-\omega[r_1+r_2] \cosh \sigma) I_{2\lambda+1}(2\omega\sqrt{r_1 r_2} \sinh \sigma) d\sigma \\
&\quad (4.3.7)
\end{aligned}$$

$$= (1/2\omega) \frac{\Gamma(\lambda+1-\nu)}{\Gamma(2\lambda+2)} \frac{1}{r_1 r_2} M_{\nu, \lambda+\frac{1}{2}}(2\omega r_<) W_{\nu, \lambda+\frac{1}{2}}(2\omega r_>) \quad (4.3.8)$$

The off-diagonal terms can be simply calculated using (4.2.13b) and (4.2.15b), but the matrix elements, which are double Laplace transforms calculated in the next chapter, are simple to calculate without actually deriving explicit forms. However, the Sturmian expansion is of interest since it is not quite what one might expect. Using the relations (2.3.29) and (2.3.30) derived in Chapter II, together with the series expansion for the delta function (3.1.20) found in the last chapter, it is not difficult to see that

$$\begin{aligned}
h^{21}(r_1, r_2) &= h^{12}(r_2, r_1) \\
&= (1-\kappa^2)/(2\hbar c\gamma) \left[ \delta(r_1-r_2)/\sqrt{r_1 r_2} + (2\omega)^{2\gamma+1} r_1^{\gamma-1} r_2^\gamma \right. \\
&\quad \times e^{-\omega(r_1+r_2)} \sum_{k=0}^{\infty} \frac{(k+1)! (\gamma+k+1-\nu)^{-1}}{\Gamma(2\gamma+1+k)} L_{k+1}^{2\gamma-1}(2\omega r_1) L_k^{2\gamma+1}(2\omega r_2) \left. \right] \quad (4.3.9)
\end{aligned}$$

We see first of all that  $h^{ij}(r_1, r_2) = h^{ji}(r_2, r_1)$ . Thus, in spite of the seemingly asymmetrical defining equations for the radial Dirac-Coulomb Green functions they are nonetheless symmetrical in  $r_1$  and  $r_2$ . Next we notice that the off-diagonal terms are not simple Sturmian expansions.



The delta function appearing in (4.3.9) is required for the correct calculation of the matrix elements.

A Sturmian form of the radial Dirac-Coulomb Green function was obtained previously<sup>18</sup> by solving the second order problem. The method is quite complicated and the solution presented, while apparently equivalent to the one above, does not explicitly display the delta function. Thus the solution does not actually look like an expansion of the appropriate Sturmian wavefunctions.

We can find expressions for  $h^{12}$  and  $h^{21}$  in terms of Whittaker functions also. Using the relations given in Appendix A.1 for the derivatives of  $M$  and  $W$ , and the defining equations (4.2.13b) and (4.2.15b) we find that

$$\begin{aligned}
 h^{21}(r_1, r_2) &= h^{12}(r_2, r_1) \\
 &= \frac{(1-\kappa^2)\Gamma(\gamma+1-\nu)}{2\gamma\hbar c\Gamma(2\gamma+2)} \frac{1}{r_1 r_2} \left[ 2\gamma(2\gamma+1)\theta(r_2-r_1)M_{\nu, \gamma-\frac{1}{2}}(2\omega r_1)W_{\nu, \gamma+\frac{1}{2}}(2\omega r_2) \right. \\
 &\quad \left. - (\nu+\gamma)\theta(r_1-r_2)W_{\nu, \gamma-\frac{1}{2}}(2\omega r_1)M_{\nu, \gamma+\frac{1}{2}}(2\omega r_2) \right], \quad (4.3.10)
 \end{aligned}$$

where  $\theta(r)$  is the unit Heaviside function. Notice that no delta function appears in this expression. Notice also the lack of symmetry in the coefficients multiplying the Whittaker functions.

This last expression for the off-diagonal elements is in direct contradiction to those obtained by Wong and Yeh<sup>41</sup>. Their extension of Biedenharn's method leads them to equations (4.2.10), though they are wrong in asserting that these equations hold for the (non-transformed) radial Green functions. However, they then proceed to a solution as an

expansion in eigenfunctions of the homogeneous equations. This method, essentially given by (1.4) is only applicable when the energy variable is multiplying the identity. Obviously, in (4.2.10) the energy variable  $\epsilon$  appears on and off the diagonal and thus Wong (and Yeh's method fails.

#### 4.4: REDUCTION TO THE NONRELATIVISTIC LIMIT

To complete the analysis I present a brief examination of the nonrelativistic limit of the Dirac-Coulomb Green function we have just calculated. It will be useful to express the original radial functions in terms of the radial functions we have obtained. Thus, inverting (4.2.11) we find

$$\begin{bmatrix} g^{11} & g^{12} \\ g^{21} & g^{22} \end{bmatrix} = \frac{1}{(1-\kappa^2)^2} \begin{bmatrix} h^{11} - \kappa(h^{12} + h^{21}) + \kappa^2 h^{22} & -\kappa(h^{11} + h^{22}) + h^{12} + \kappa^2 h^{21} \\ -\kappa(h^{11} + h^{22}) + \kappa^2 h^{12} + h^{21} & \kappa^2 h^{11} - \kappa(h^{12} + h^{21}) + h^{22} \end{bmatrix} \quad (4.4.1)$$

As in the reduction of the Dirac-Coulomb wavefunctions to their nonrelativistic limits, two separate situations obtain, depending on the sign of  $\kappa$ . (It will be useful at this point to refer to equations (2.2.36).) We use the Sturmian expansion throughout.

When  $\kappa = |\kappa|$ , we set  $\kappa = \ell$ ,  $\omega = 1/a\nu$  and note

$$\kappa \approx -\alpha Z/2\ell, \quad 1-\kappa^2 \approx 1, \quad \epsilon\kappa + \epsilon_0\gamma \approx 2\ell/a\alpha Z, \quad \epsilon\kappa - \epsilon_0\gamma \approx \alpha Z(\nu^2 - \ell^2)/2a\nu^2$$

and  $\gamma \simeq \ell$ . Then the lowest order term in  $\alpha Z$  is  $g^{11}$  and is the nonrelativistic limit of  $h^{11}$ , which is itself easily seen to equal  $g_\ell(\nu)$ . Hence, for  $\kappa = |\kappa| = \ell$ ,

$$\begin{bmatrix} g^{11} & g^{12} \\ g^{21} & g^{22} \end{bmatrix} \simeq \begin{bmatrix} g_\ell & 0 \\ 0 & 0 \end{bmatrix} \quad (4.4.2)$$

When  $\kappa = -|\kappa|$ , we set  $\kappa = -\ell - 1$ ,  $\omega \simeq 1/a\nu$ , and note

$$K \simeq 2(\ell+1)/\alpha Z, \quad 1-K^2 \simeq -4(\ell+1)^2/\alpha^2 Z^2,$$

$$\epsilon\kappa + \epsilon_0\gamma \simeq -\alpha Z(\nu - \ell - 1)(\nu + \ell + 1)/[2a(\ell+1)\nu^2], \quad \epsilon\kappa - \epsilon_0\gamma \simeq -2(\ell+1)/(a\alpha Z)$$

and  $\gamma \simeq \ell + 1$ . The lowest order term in  $\alpha Z$  is again  $g^{11}$  but is now the nonrelativistic limit of  $h^{22}$ , which again is equal to  $g_\ell(\nu)$ . Hence, for  $\kappa = -|\kappa| = -\ell - 1$ , we arrive at equation (4.4.2) again.

Thus, in the nonrelativistic limit, all terms in the  $2 \times 2$  matrix of radial Dirac-Coulomb Green functions but the leading diagonal term vanish, and the nonvanishing element is just the radial Schrodinger-Coulomb Green function as we might have expected.

## CHAPTER 5 : THE DOUBLE LAPLACE TRANSFORMS OF THE COULOMB GREEN FUNCTIONS.

### 5.0 : INTRODUCTION

Matrix elements of both the nonrelativistic and relativistic Coulomb Green functions can be calculated once we know the double Laplace transforms (DLT) of the radial functions. Previously only a very specific case of the DLT has been calculated<sup>42</sup>. In keeping with the overall philosophy of this dissertation I will present the most general results I can. Thus future calculations involving the Coulomb Green functions will not require the calculation of another specific case. From a numerical standpoint, it may be wisest to have as many different forms of the same matrix element as possible in order to facilitate the choice of the most rapidly convergent and stable solution for the particular problem one is analysing.

### 5.1 : DLT'S OF THE SCHRODINGER-COULOMB GREEN FUNCTION.

The Schrodinger-Coulomb radial wavefunctions involve only integer powers of  $r$ . For this reason we will consider here the general DLT of  $g_\ell(r_1, r_2; \nu)$  defined to be

$$K_{n_1 n_2}^\ell(p_1, p_2; \nu) = \hbar^2 / (2m) \int_0^\infty r_1^{n_1} r_2^{n_2} e^{-(p_1 r_1 + p_2 r_2) / a \nu} g_\ell(r_1, r_2; \nu) dr_1 dr_2 \quad (5.1.1)$$

where  $n_1$  and  $n_2$  are integers. The special case, where  $n_1 = n_2 = \ell + 1$  is well

known, and can be written<sup>42</sup>

$$K_{\ell+1, \ell+1}^{\ell}(p_1, p_2; \nu) = 2^{2\ell+1} (a\nu)^{2\ell+3} [(1+p_1)(1+p_2)]^{-2\ell-2} \\ \times \frac{(2\ell+1)!}{(\ell-\nu+1)!} {}_2F_1(2\ell+2, \ell-\nu+1; \ell-\nu+2; \left[\frac{1-p_1}{1+p_1}\right] \left[\frac{1-p_2}{1+p_2}\right]) \quad (5.1.2)$$

This result will be useful for checking the more general calculations which follow.

We begin our derivations of the various representations of  $K_{n_1 n_2}^{\ell}$  by considering the form of  $g_{\ell}$  given in equation (3.2.5) (form [C]). Noting that

$$J_{n_1 n_2}^{\ell}(u_1, u_2; \sigma) \equiv \int_0^{\infty} x_1^{n_1-\frac{1}{2}} x_2^{n_2-\frac{1}{2}} e^{-u_1 x_1 - u_2 x_2} I_{2\ell+1}(2\sqrt{\sigma x_1 x_2}) dx_1 dx_2 \\ = \frac{(n_1+\ell)! (n_2+\ell)!}{(2\ell+1)!} \sigma^{\ell+\frac{1}{2}} u_1^{-n_1-\ell-1} u_2^{-n_2-\ell-1} {}_2F_1(n_1+\ell+1, n_2+\ell+1; 2\ell+2; \sigma/(u_1 u_2)) \quad ,$$

we find

$$K_{n_1 n_2}^{\ell}(p_1, p_2; \nu) = \int_0^{\infty} (1-s)^{-\nu-\frac{1}{2}} s^{-1} J_{n_1 n_2}^{\ell} \left[ \frac{p_1-1+2/s}{a\nu}, \frac{p_2-1+2/s}{a\nu}, \frac{4(1-s)}{a^2 \nu^2 s^2} \right] ds \\ = (a\nu/2)^{n_1+n_2+1} \sum_{k=0}^{\infty} \frac{(n_1+\ell+k)! (n_2+\ell+k)!}{(2\ell+1+k)! k!} \int_0^1 s^{n_1+n_2} (1-s)^{\ell+k-\nu} \\ \times \left[ 1 - \frac{s}{2}(1-p_1) \right]^{-n_1-\ell-1-k} \left[ 1 - \frac{s}{2}(1-p_2) \right]^{-n_2-\ell-1-k} ds \quad (5.1.3)$$

Now, Appell's hypergeometric function of two variables of the first kind,  $F_1$  is the only two-dimensional hypergeometric function which can be represented by a single integral<sup>43,44</sup>, this being

$$\frac{\Gamma(\alpha)\Gamma(\gamma-\alpha)}{\Gamma(\gamma)} F_1(\alpha, \beta, \beta'; \gamma, x, y) = \int_0^1 u^{\alpha-1} (1-u)^{\gamma-\alpha-1} (1-ux)^{-\beta} (1-uy)^{-\beta'} du. \quad (5.1.4)$$

Hence,

$$\begin{aligned} K_{n_1 n_2}^\ell(p_1, p_2; \nu) &= (a\nu/2)^{n_1+n_2+1} (n_1+n_2)! \\ &\times \sum_{k=0}^{\infty} \frac{(n_1+\ell+k)! (n_2+\ell+k)! \Gamma(\ell+k+1-\nu)}{(2\ell+1+k)! k! \Gamma(\ell+k+2+n_1+n_2-\nu)} \\ &\times F_1(n_1+n_2+1; k+n_1+\ell+1, k+n_2+\ell+1; k+n_1+n_2+\ell+2-\nu; \left[\frac{1-p_1}{2}\right] \left[\frac{1-p_2}{2}\right]) . \end{aligned} \quad (5.1.5)$$

When the second two parameters in  $F_1$  are integers it is possible to express it as two finite sums of ordinary hypergeometric functions, a fact which was noted in ref. 46 though not explicitly stated. This interesting result is derived in Appendix B.2 ; here we are content to state the result.

$$\begin{aligned} F_1(\alpha; m, m'; \gamma; x, y) &= (-1)^m x^m y^m (x-y)^{-m-m'} \\ &\times \left[ \sum_{i=1}^m \frac{(m+m'-i-1)!}{(m-i)!(m'-1)!} (x-y)^i y^{-i} {}_2F_1(\alpha, i; \gamma; x) \right. \\ &\left. + \sum_{i=1}^{m'} \frac{(m+m'-i-1)!}{(m'-i)!(m-1)!} (y-x)^i x^{-i} {}_2F_1(\alpha, i; \gamma; y) \right] \end{aligned} \quad (5.1.6)$$

Reordering the three sums in (5.1.5) gives

$$\begin{aligned} K_{n_1 n_2}^\ell(p_1, p_2; \nu) &= (a\nu/2)^{n_1+n_2+1} \sum_{m_1, m_2} \frac{(n_1+n_2+m_1+m_2)! (n_1+\ell+m_1)! (n_2+\ell+m_2)!}{\Gamma(\ell+n_1+n_2+m_1+m_2+2-\nu) m_1! m_2!} \\ &\times \frac{\Gamma(\ell+1-\nu)}{(2\ell+1)!} \left[\frac{1-p_1}{2}\right]^{m_1} \left[\frac{1-p_2}{2}\right]^{m_2} {}_3F_2 \left[ \begin{matrix} n_1+m_1+\ell+1, & n_2+m_2+\ell+1, & \ell-\nu+1 \\ \ell+n_1+n_2+m_1+m_2+2-\nu, & 2\ell+2 \end{matrix} ; 1 \right] . \end{aligned} \quad (5.1.7)$$

The generalized hypergeometric function of unit argument,  ${}_3F_2(1)$  has interesting properties which have been known for some time<sup>43,45</sup>. In particular, it is possible to transform the arguments among themselves to derive other, equal forms. Thus it can be shown that

$${}_3F_2\left[\begin{matrix} a & b & c \\ e & f \end{matrix}; 1\right] = \frac{\Gamma(s)\Gamma(e)\Gamma(f)}{\Gamma(e-c)\Gamma(s+c)\Gamma(f)} {}_3F_2\left[\begin{matrix} f-b & f-a & c \\ s+c & f \end{matrix}; 1\right] \quad (5.1.8)$$

where  $s=e+f-a-b-c$ . [This is equivalent to  $F_p(0;4,5)=F_p(0;3,5)$  in Bailey's notation<sup>43</sup>.] Hence

$${}_3F_2\left[\begin{matrix} n_1+m_1+\ell+1, & n_2+m_2+\ell+1, & \ell-\nu+1 \\ \ell+n_1+n_2+m_1+m_2+2-\nu, & 2\ell+2 \end{matrix}; 1\right] = \frac{\Gamma(\ell+n_1+n_2+m_1+m_2+2-\nu)}{(n_1+n_2+m_1+m_2)! \Gamma(\ell-\nu+2)} {}_3F_2\left[\begin{matrix} \ell+1-n_1-m_1, & \ell+1-n_2-m_2, & \ell-\nu+1 \\ 2\ell+2 & \ell-\nu+2 \end{matrix}; 1\right] \quad (5.1.9)$$

and this allows us to transform (5.1.7) into

$$K_{n_1 n_2}^\ell(p_1, p_2; \nu) = (a\nu/2)^{n_1+n_2+1} \sum_{k=0}^{\infty} \frac{F_{k,\ell}^{n_1}(p_1) F_{k,\ell}^{n_2}(p_2)}{(2\ell+1+k)! k! (\ell+k+1-\nu)} \quad (5.1.10)$$

$$\text{where } F_{k,\ell}^n(p) = \sum_{m=0}^{\infty} (n+m+\ell)! (\ell+1-n-m)_k / m! \left[\frac{1-p}{2}\right]^m \quad (5.1.11)$$

and  $(x)_0 = 1$ ,  $(x)_k = x(x+1)\dots(x+k-1)$ . The  $F_{k,\ell}^n(p)$  functions can always be written as finite polynomials, the number of terms in which is never greater than  $\max\{n+\ell, n-\ell\}$ . Thus we have in (5.1.10) an expression for  $K_{n_1 n_2}^\ell$  consisting of a finite number of singly infinite sums. Specifically we have three cases:

(a)  $\ell \geq n$ 

$$F_{k,\ell}^n(p) = (\ell-n+k)!(n+\ell)!/(\ell-n)! {}_2F_1(-\ell+n, n+\ell+1; -\ell-k+n; \frac{1-p}{2}) \\ - \left[\frac{1-p}{2}\right]^{\ell-n} \left[\frac{p-1}{p+1}\right]^{k+1} \frac{(2\ell+1+k)!k!}{(\ell-n+1+k)!} {}_2F_1(-n-\ell, k+1; \ell-n+k+2; \left[\frac{p-1}{p+1}\right]) ; \quad (5.1.12a)$$

(b)  $n \geq \ell+1, k < n-\ell$ 

$$F_{k,\ell}^n(p) = (-1)^k \frac{(n+\ell)!(n-\ell-1)!}{(n-\ell-1-k)!} \left[\frac{2}{1+p}\right]^{n+\ell+1} {}_2F_1(n+\ell+1, -k; n-\ell-k; \left[\frac{p-1}{p+1}\right]) ; \quad (5.1.12b)$$

(c)  $n \geq \ell+1, k \geq n-\ell$ 

$$F_{k,\ell}^n = (-1)^k \frac{(2\ell+1+k)!k!}{(k+\ell+1-n)!} \left[\frac{1-p}{1+p}\right]^{k+\ell+1} \frac{2^{2n}}{(1-p^2)^n} {}_2F_1(-n-\ell, \ell+1-n; k+2+\ell-n; \frac{1-p}{2}). \quad (5.1.12c)$$

Notice that although we have polynomials of order  $k$  in (b), in that case  $k$  itself is bounded by  $n$ . The special case is retrieved once we notice that

$$F_{k,\ell}^{\ell+1}(p) = (2\ell+1+k)! 2^{2\ell+2}/(1+p)^{2\ell+2} \left[\frac{p-1}{p+1}\right]^k$$

from which (5.1.2) follows.

The second transformation of the  ${}_3F_2(1)$  hypergeometric series we use is known as Thomae's Theorem<sup>45</sup> and states that

$${}_3F_2\left[\begin{matrix} a & b & c \\ e & f \end{matrix}; 1\right] = \frac{\Gamma(e)\Gamma(f)\Gamma(s)}{\Gamma(a)\Gamma(s+b)\Gamma(s+c)} {}_3F_2\left[\begin{matrix} e-a & f-a & s \\ s+b & s+c \end{matrix}; 1\right] \quad (5.1.13)$$

where, as before  $s=e+f-a-b-c$ , and from which we deduce that



$${}_3F_2 \left[ \begin{matrix} n_1+m_1+\ell+1, n_2+m_2+\ell+1, \ell-\nu+1 \\ \ell+n_1+n_2+m_1+m_2+2-\nu, 2\ell+2 \end{matrix} ; 1 \right] =$$

$$\frac{(2\ell+1)!\Gamma(\ell+n_1+n_2+m_1+m_2+2-\nu)}{\Gamma(\ell-\nu+1)(\ell+n_1+m_1+1)!(\ell+n_2+m_2+1)!} {}_3F_2 \left[ \begin{matrix} n_1+n_2+m_1+m_2+1, \ell+1-\nu, 1 \\ \ell+n_1+m_1+2, \ell+n_2+m_2+2 \end{matrix} ; 1 \right].$$

(5.1.14)

From this we deduce a further representation of the DLT written now in terms of  $F_2$ , an Appell hypergeometric function of two variables of the second kind<sup>44</sup>:

$$K_{n_1 n_2}^\ell(p_1, p_2; \nu) = (a\nu/2)^{n_1+n_2+1} (\ell+n_1)!(\ell+n_2)!/\Gamma(\ell+1+\nu)$$

$$\times \sum_{k=0}^{\infty} \frac{(n_1+n_2+k)!\Gamma(\ell+1+\nu+k)}{(\ell+n_1+k+1)!(\ell+n_2+k+1)!}$$

$$\times F_2(n_1+n_2+k+1; \ell+n_1+1, \ell+n_2+1; \ell+n_1+k+2, \ell+n_2+k+2; \left[\frac{1-p_1}{2}\right] \left[\frac{1-p_2}{2}\right]) \quad (5.1.15)$$

Notice that the parameters of the  $F_2$  hypergeometric function do not depend on the energy variable,  $\nu$ . Notice further that we can deduce the special case,  $n_1 = n_2 = \ell+1$ , by appealing to the transformation<sup>44</sup>

$$F_2(\alpha; \beta, \beta'; \alpha, \alpha; x, y) = (1-x)^{-\beta} (1-y)^{-\beta'} {}_2F_1(\beta, \beta'; \alpha; xy/[(1-x)(1-y)]) \quad (5.1.16)$$

We can also calculate  $K_{n_1 n_2}^\ell$  using the Sturmian expansion for  $g_\ell$  (representation [A], (3.2.1)). In this calculation the integrals over  $r_1$  and  $r_2$  formally separate giving

$$K_{n_1 n_2}^\ell(p_1, p_2; \nu) = (2/a\nu)^{2\ell+1} \sum_{k=0}^{\infty} k! / [(2\ell+1+k)!(\ell+1+k-\nu)]$$

$$\times \int_0^\infty r_1^{\ell+n_1} e^{-(p_1+1)r_1/a\nu} L_k^{2\ell+1} \left[ \frac{2r_1}{a\nu} \right] dr_1 \times \int_0^\infty r_2^{\ell+n_2} e^{-(p_2+1)r_2/a\nu} L_k^{2\ell+1} \left[ \frac{2r_2}{a\nu} \right] dr_2$$

Now, noting that

$$\begin{aligned} & \int_0^\infty r^{\ell+n} e^{-(p+1)r/a\nu} L_k^{2\ell+1}(2r/a\nu) dr \\ &= (a\nu)^{\ell+n+1} (\ell+n+k)!/k! \left[ \frac{p-1}{p+1} \right]^k (p+1)^{-\ell-n-1} {}_2F_1(-k, \ell+1-n; -\ell-n-k, \frac{p+1}{p-1}) \end{aligned} \quad (5.1.17)$$

leads us to the following representation:

$$\begin{aligned} K_{n_1 n_2}^\ell(p_1, p_2; \nu) &= 2^{2\ell+1} (a\nu)^{n_1+n_2+1} (p_1+1)^{-\ell-n_1-1} (p_2+1)^{-\ell-n_2-1} \\ &\times \sum_{k=0}^\infty \frac{(\ell+n_1+k)! (\ell+n_2+k)!}{(2\ell+1+k)! k! (\ell+1+k-\nu)} \left[ \frac{p_1-1}{p_1+1} \right]^k \left[ \frac{p_2-1}{p_2+1} \right]^k \\ &\times {}_2F_1(-k, \ell+1-n_1; -\ell-n_1-k, \frac{p_1+1}{p_1-1}) {}_2F_1(-k, \ell+1-n_2; -\ell-n_2-k, \frac{p_2+1}{p_2-1}) \end{aligned} \quad (5.1.18)$$

If  $n_1$  or  $n_2$  are greater than  $\ell+1$  then the respective hypergeometric functions become polynomials whose degree is independent of  $k$  for large  $k$ . For  $n_1=n_2=\ell+1$  the hypergeometric functions disappear and our special case is once again verified.

Our last expression for  $K_{n_1 n_2}^\ell$  is obtained with the use of the representation of  $g_\ell$  in terms of Bessel functions (form [F], (3.2.10)). We again find that the integration over variables with different subscripts separates: Indeed, on changing the order of integration we find

$$\begin{aligned}
K_{n_1 n_2}^\ell(p_1, p_2; \nu) &= \sum_{k=0}^{\infty} 1/[(2\ell+1+k)!k!(\ell+1+k-\nu)] \\
&\times \int_0^\infty s_1^{k+\ell+\frac{1}{2}} e^{-s_1} \int_0^\infty r_1^{n_1-\frac{1}{2}} e^{-(p_1-1)r_1/a\nu} J_{2\ell+1}(2\sqrt{2r_1 s_1/a\nu}) dr_1 ds_1 \\
&\times \int_0^\infty s_2^{k+\ell+\frac{1}{2}} e^{-s_2} \int_0^\infty r_2^{n_2-\frac{1}{2}} e^{-(p_2-1)r_2/a\nu} J_{2\ell+1}(2\sqrt{2r_2 s_2/a\nu}) dr_2 ds_2 \quad (5.1.19)
\end{aligned}$$

Now

$$\begin{aligned}
&\int_0^\infty r^{n-\frac{1}{2}} e^{-(p-1)r/a\nu} J_{2\ell+1}(2\sqrt{2rs/a\nu}) dr \\
&= (a\nu)^{n+\frac{1}{2}} \frac{(n+\ell)!}{(2\ell+1)!} (2s)^{\ell+\frac{1}{2}} (p-1)^{-\ell-n-1} {}_1F_1(n+\ell+1; 2\ell+2; \frac{2s}{1-p}) \quad (5.1.20)
\end{aligned}$$

and

$$\begin{aligned}
&\int_0^\infty s^{k+2\ell+1} e^{-s} {}_1F_1(n+\ell+1; 2\ell+2; \frac{2s}{1-p}) \\
&= (2\ell+k+1)! \left[ \frac{p-1}{p+1} \right]^{n+\ell+1} {}_2F_1(n+\ell+1, -k; 2\ell+2; \frac{2}{1+p}) \quad (5.1.21)
\end{aligned}$$

so that

$$\begin{aligned}
K_{n_1 n_2}^\ell(p_1, p_2; \nu) &= (a\nu)^{n_1+n_2+1} 2^{2\ell+1} \frac{(n_1+\ell)!(n_2+\ell)!}{[(2\ell+1)!]^2} \\
&\times (p_1+1)^{-n_1-\ell-1} (p_2+1)^{-n_2-\ell-1} \\
&\times \sum_{k=0}^{\infty} \frac{(2\ell+1+k)!}{(\ell+1+k-\nu)k!} {}_2F_1(-k, n_1+\ell+1; 2\ell+2; \frac{2}{1+p_1}) {}_2F_1(-k, n_2+\ell+1; 2\ell+2; \frac{2}{1+p_2}) \quad (5.1.22)
\end{aligned}$$

When  $n_1 = n_2 = \ell + 1$  this final representation immediately reduces to the special case, (5.1.12).

## 5.2 : DLT'S OF THE DIRAC-COULOMB GREEN FUNCTION

The double Laplace transforms of the radial part of the Dirac-Coulomb Green function can be found quite quickly by analogy to the preceding discussion. In fact, we need only really consider the DLT's of the diagonal elements, since the DLT's of the off-diagonal elements are simply related to them. So, we concentrate on calculating

$$K_{\mu_1 \mu_2}^\lambda(p_1, p_2; \omega) = \int_0^\infty r_1^{\mu_1} r_2^{\mu_2} e^{-(p_1 r_1 + p_2 r_2) \omega} h(r_1, r_2; \lambda, \omega) dr_1 dr_2 \quad (5.2.1)$$

where the  $\mu$ 's are not necessarily integers, and we have defined  $h$  in the last chapter (4.3.3).

Much of the analysis of the previous section is still applicable. Indeed, that is the power of the treatment of the Dirac-Coulomb Green function presented in the last chapter. The main difference is that many of the parameters involved in the calculation are no longer integers. Thus some of the compact expressions presented in the last section for the DLT of  $g_\ell$  will not be possible. However, there are several expressions which do still obtain, in somewhat modified form, and they are presented now. The results will be presented without proof; the proofs consist of simple generalizations of those given in Section 5.1.

As before we begin with the integral representation of  $h$ , equation (4.3.6). Then we get

$$\begin{aligned}
K_{\mu_1 \mu_2}^{\lambda}(p_1, p_2; \omega) &= (1/2\omega)^{\mu_1 + \mu_2 + 1} \Gamma(\mu_1 + \mu_2 + 1) \\
&\times \sum_{k=0}^{\infty} \frac{\Gamma(\lambda + \mu_1 + k + 1) \Gamma(\lambda + \mu_2 + k + 1) \Gamma(\lambda + k + 1 - \nu)}{\Gamma(2\lambda + 2 + k) k! \Gamma(\lambda + \mu_1 + \mu_2 + k + 2 - \nu)} \\
&\times F_1(\mu_1 + \mu_2 + 1; \lambda + \mu_1 + k + 1, \lambda + \mu_2 + k + 1; \lambda + \mu_1 + \mu_2 + k + 2 - \nu; \left[\frac{1-p_1}{2}\right], \left[\frac{1-p_2}{2}\right]) \quad (5.2.2)
\end{aligned}$$

$$\begin{aligned}
&= (1/2\omega)^{\mu_1 + \mu_2 + 1} \\
&\times \sum_{m_1, m_2}^{\infty} \frac{\Gamma(\mu_1 + \mu_2 + m_1 + m_2 + 1) \Gamma(\lambda + \mu_1 + m_1 + 1) \Gamma(\lambda + \mu_2 + m_2 + 1) \Gamma(\lambda + 1 - \nu)}{\Gamma(\lambda + \mu_1 + \mu_2 + m_1 + m_2 + 2 - \nu) \Gamma(2\lambda + 2) m_1! m_2!} \\
&\times \left[\frac{1-p_1}{2}\right]^{m_1} \left[\frac{1-p_2}{2}\right]^{m_2} {}_3F_2\left[\begin{matrix} \mu_1 + m_1 + \lambda + 1, \mu_2 + m_2 + \lambda + 1, \lambda + 1 - \nu \\ \lambda + \mu_1 + \mu_2 + m_1 + m_2 + 2 - \nu, 2\lambda + 2 \end{matrix}; 1\right] \quad (5.2.3)
\end{aligned}$$

$$\begin{aligned}
&= (1/2\omega)^{\mu_1 + \mu_2 + 1} \Gamma(\lambda + \mu_1 + 1) \Gamma(\lambda + \mu_2 + 1) / \Gamma(\lambda + 1 + \nu) \\
&\times \sum_{k=0}^{\infty} \frac{\Gamma(\mu_1 + \mu_2 + k + 1) \Gamma(\lambda + 1 + \nu + k)}{\Gamma(\lambda + \mu_1 + k + 2) \Gamma(\lambda + \mu_2 + k + 2)} \\
&\times F_2(\mu_1 + \mu_2 + k + 1; \lambda + \mu_1 + 1, \lambda + \mu_2 + 1; \lambda + \mu_1 + k + 2, \lambda + \mu_2 + k + 2; \left[\frac{1-p_1}{2}\right], \left[\frac{1-p_2}{2}\right]) \quad (5.2.4)
\end{aligned}$$

The Sturmiian expansion (4.3.3) is again useful for calculating the DLT's. In fact, the off-diagonal elements can also be treated in this form.

$$\begin{aligned}
K_{\mu_1 \mu_2}^{\lambda}(p_1, p_2; \omega) &= 2^{2\lambda + 1} \omega^{-\mu_1 - \mu_2 - 1} (p_1 + 1)^{-\mu_1 - \lambda - 1} (p_2 + 1)^{-\mu_2 - \lambda - 1} \\
&\times \sum_{k=0}^{\infty} \frac{\Gamma(\mu_1 + \lambda + k + 1) \Gamma(\mu_2 + \lambda + k + 1)}{\Gamma(2\lambda + 2 + k) k! (\lambda + 1 + k - \nu)} \left[\frac{p_1 - 1}{p_1 + 1}\right]^k \left[\frac{p_2 - 1}{p_2 + 1}\right]^k \\
&\times {}_2F_1(-k, \lambda + 1 - \mu_1; -\mu_1 - \lambda - k; \frac{p_1 + 1}{p_1 - 1}) {}_2F_1(-k, \lambda + 1 - \mu_2; -\mu_2 - \lambda - k; \frac{p_2 + 1}{p_2 - 1}) \quad (5.2.5)
\end{aligned}$$

and

$$\begin{aligned}
 K_{\mu_1 \mu_2}^{\gamma}(p_1, p_2; \omega) &\equiv \int_0^\infty r_1^{\mu_1} r_2^{\mu_2} e^{-(r_1 p_1 + r_2 p_2) \omega} h^{21}(r_1, r_2) dr_1 dr_2 \\
 &= (1-\lambda^2)/(2\hbar c \gamma) (1/\omega)^{\mu_1 + \mu_2} \\
 &\left[ (p_1 + p_2)^{-\mu_1 - \mu_2} \Gamma(\mu_1 + \mu_2) + 2^{2\gamma+1} (p_1 + 1)^{-\mu_1 - \gamma} (p_2 + 1)^{-\mu_2 - \gamma - 1} \right. \\
 &\quad \times \sum_{k=0}^{\infty} \frac{\Gamma(\mu_1 + \gamma + k + 1) \Gamma(\mu_2 + \gamma + k + 1)}{\Gamma(2\gamma + 1 + k) (\gamma + k + 1 - \nu) k!} \left[ \frac{p_1 - 1}{p_1 + 1} \right]^{k+1} \left[ \frac{p_2 - 1}{p_2 + 1} \right]^k \\
 &\quad \times {}_2F_1(-k-1, \gamma - \mu_1; -\mu_1 - \gamma - k; \frac{p_1 + 1}{p_1 - 1}) {}_2F_1(-k, \gamma - \mu_2 + 1; -\mu_2 - \gamma - k; \frac{p_2 + 1}{p_2 - 1}) \left. \right] \quad (5.2.6)
 \end{aligned}$$

The last two expressions are all that is needed to determine the relativistic matrix elements of the Dirac-Coulomb Green function.

Finally, there is a representation of  $K$  based on the form of  $h$  given by (4.3.4). The analysis is the same as before.

$$\begin{aligned}
 K_{\mu_1 \mu_2}^{\lambda}(p_1, p_2; \omega) &= 2^{\lambda+1} \omega^{-\mu_1 - \mu_2 - 1} \\
 &\times (p_1 + 1)^{-\lambda - \mu_1 - 1} (p_2 + 1)^{-\lambda - \mu_2 - 1} \frac{\Gamma(\mu_1 + \lambda + 1) \Gamma(\mu_2 + \lambda + 1)}{[\Gamma(2\lambda + 2)]^2} \sum_{k=0}^{\infty} \frac{\Gamma(2\lambda + 2 + k)}{k! (\lambda + 1 + k)} \\
 &\times {}_2F_1(\mu_1 + \lambda + 1, -k; 2\lambda + 2; \frac{2}{p_1 + 1}) {}_2F_1(\mu_2 + \lambda + 1, -k; 2\lambda + 2; \frac{2}{p_2 + 1}) \quad (5.2.7)
 \end{aligned}$$

### 5.3 : A GENERALIZED DLT OF THE RADIAL COULOMB GREEN FUNCTIONS.

In this section we begin by considering a very specific 'generalization' of the DLT of the radial Schrodinger-Coulomb Green function, namely

$$\begin{aligned} \bar{K}_{n_1 n_2}^{\ell}(p_1, p_2; k_1, k_2; \nu) = & \hbar^2/2m \int_0^{\infty} r_1^{n_1} e^{-p_1 r_1/a\nu} j_{\ell}(k_1 r_1/a\nu) \\ & \times g_{\ell}(r_1, r_2; \nu) j_{\ell}(k_2 r_2/a\nu) r_2^{n_2} e^{-p_2 r_2/a\nu} dr_1 dr_2, \end{aligned} \quad (5.3.1)$$

where  $j_{\ell}$  is a spherical Bessel function defined by<sup>38</sup>

$$j_{\ell}(\sigma) = \sqrt{\pi/2\sigma} J_{\ell+\frac{1}{2}}(\sigma) \quad (5.3.2)$$

This transform will be found to be of interest in the later Chapter on two-photon transitions. It is also intimately related to the Fourier transform of the Green function into momentum space. There  $k_1$  and  $k_2$  are just the magnitudes of the momentum space vectors.

We have, in fact, already found this transform. By expanding the spherical Bessel functions in power series we find immediate use for our DLT's discussed in a previous section. However, we can find much more compact expressions for  $\bar{K}$  than those a power series expansion would yield. Specifically we will calculate  $\bar{K}_{11}^{\ell}$  for which a particularly simple form exists, and which has furthermore been considered by other authors<sup>5</sup>. We begin introducing representation [F], (3.2.10) for the radial Green function into (5.3.1) with  $n_1=n_2=1$  and interchanging formally the order of integration.



$$\begin{aligned}
K_{11}^{\ell}(p_1, p_2; k_1, k_2; \nu) &= \int_0^{\infty} e^{-s_1-s_2} \sum_{k=0}^{\infty} \frac{(s_1 s_2)^{k+\ell+\frac{1}{2}}}{(2\ell+1+k)! k! (\ell+1+k-\nu)} \\
&\times \left[ \int_0^{\infty} \sqrt{r_1} e^{-(p_1-1)r_1/a\nu} J_{2\ell+1}(2\sqrt{2r_1 s_1}/a\nu) j_{\ell}(k_1 r_1/a\nu) dr_1 \right] \\
&\times \left[ \int_0^{\infty} \sqrt{r_2} e^{-(p_2-1)r_2/a\nu} J_{2\ell+1}(2\sqrt{2r_2 s_2}/a\nu) j_{\ell}(k_2 r_2/a\nu) dr_2 \right] ds_1 ds_2 \quad (5.3.3)
\end{aligned}$$

Now<sup>47</sup>,

$$\int_0^{\infty} e^{-q\sigma} J_{\lambda}(b\sigma) J_{2\lambda}(2\sqrt{c}\sigma) d\sigma = (q^2+b^2)^{-\frac{1}{2}} e^{-cq/(q^2+b^2)} J_{\lambda}\left[\frac{cb}{q^2+b^2}\right] \quad (5.3.4)$$

which allows us to perform the integrals over  $r_1$  and  $r_2$  immediately, giving

$$\begin{aligned}
K_{11}^{\ell}(p_1, p_2; k_1, k_2; \nu) &= \\
&\pi/2 (a\nu)^3 [k_1 k_2 ((p_1-1)^2 + k_1^2) ((p_2-1)^2 + k_2^2)]^{-\frac{1}{2}} \sum_{k=0}^{\infty} \frac{1}{(2\ell+1+k)! k! (\ell+1+k-\nu)} \\
&\times \int_0^{\infty} s_1^{k+\ell+\frac{1}{2}} e^{-s_1 a_1} J_{\ell+\frac{1}{2}}(c_1 s_1) ds_1 \int_0^{\infty} s_2^{k+\ell+\frac{1}{2}} e^{-s_2 a_2} J_{\ell+\frac{1}{2}}(c_2 s_2) ds_2, \quad (5.3.5)
\end{aligned}$$

where

$$a_i = [k_i^2 + p_i^2 - 1] / [k_i^2 + (p_i - 1)^2] \quad \text{and} \quad c_i = 2k_i / [k_i^2 + (p_i - 1)^2]. \quad (5.3.6)$$

The integrals over  $s_1$  and  $s_2$  can be calculated in several different ways. I present here a result which can be shown to have interesting consequences for the Dirac wavefunctions in momentum space; the full integration is

performed in Appendix B.3.

$$\begin{aligned}
 \int_0^\infty s^{k+\ell+\frac{1}{2}} e^{-as} J_{\ell+\frac{1}{2}}(cs) ds &= \sqrt{2c/\pi} \int_0^\infty s^{k+\ell+1} e^{-as} j_\ell(cs) ds \\
 &= \sqrt{2c/\pi} \frac{(k+2\ell+1)!k!}{(k+\ell+1)!} (-i)^{k+1} (2c)^{-\ell-1} (a^2+c^2)^{-k-1} \\
 &\times \left[ (ia-c)^{k+1} {}_2F_1(-\ell, k+1; \ell+k+2; \frac{ia-c}{ia+c}) - (ia+c)^{k+1} {}_2F_1(-\ell, k+1; \ell+k+2; \frac{ia+c}{ia-c}) \right]
 \end{aligned} \tag{5.3.7}$$

$$\begin{aligned}
 &= \sqrt{2c/\pi} 2^{-\ell} (a^2+c^2)^{-\frac{1}{2}(k+1)} 1/c^{\ell+1} (a/|a|)^{k+1} \\
 &\times \sum_{i=0}^{\ell} \frac{(k+i)! (k+2\ell+1)! \theta}{(\ell+1+k+i)! (\ell-i)! i!} (-1)^i \sin [(k+2i+1)\theta]
 \end{aligned} \tag{5.3.8}$$

where  $\theta = \tan^{-1}(c/a)$ . Notice that both of these expressions are finite sums with  $\ell$  terms; thus the number of terms in the sums does not depend upon  $k$  and our final solution for  $\bar{K}_{11}$  involves effectively only one infinite sum:

$$\begin{aligned}
 \sqrt{\bar{K}_{11}(p_1, p_2; k_1, k_2; \nu)} &= (a\nu)^3 / 2^{2\ell+1} (c_1 c_2 / k_1 k_2) [(a_1^2 + c_1^2)(a_2^2 + c_2^2)]^{-\frac{1}{2}} \\
 &\times \sum_{i=0}^{\ell} \sum_{j=0}^{\ell} \begin{bmatrix} \ell \\ i \end{bmatrix} \begin{bmatrix} \ell \\ j \end{bmatrix} (-1)^{i+j} \sum_{k=0}^{\infty} \frac{(k+i)! (k+j)! (2\ell+k+1)!}{(\ell+1+i+k)! (\ell+1+j+k)! k!} (\ell+1+k-\nu)^{-1} \\
 &\times [(a_1^2 + c_1^2)^{\frac{1}{2}} (a_2^2 + c_2^2)^{\frac{1}{2}}]^{-k} \sin [(k+2i+1)\theta_1] \sin [(k+2j+1)\theta_2],
 \end{aligned} \tag{5.3.9}$$

where  $\theta_i = \tan^{-1}(c_i/a_i)$ .

Perhaps a more familiar form of the preceding integral is that involving Gegenbauer polynomials (again the integration is performed in Appendix B.3):

$$\begin{aligned}
& \int_0^\infty s^{k+\ell+\frac{1}{2}} e^{-as} J_{\ell+\frac{1}{2}}(cs) ds \\
&= \sqrt{2c/\pi} \, k! \ell! (2c)^\ell (a^2+c^2)^{-\ell-1-k/2} C_k^{\ell+1}(a/(a^2+c^2)^{\frac{1}{2}}) \quad (5.3.10)
\end{aligned}$$

Thus

$$\begin{aligned}
& \bar{K}_{11}^\ell(p_1, p_2; k_1, k_2; \nu) = \\
& (a\nu)^3 / (4k_1 k_2) (2c_1/[a_1^2+c_1^2])^{\ell+1} (2c_2/[a_2^2+c_2^2])^{\ell+1} \sum_{k=0}^{\infty} \frac{k! (\ell!)^2}{(2\ell+1+k)! (\ell+1+k-\nu)} \\
& \times [(a_1^2+c_1^2)^{\frac{1}{2}} (a_2^2+c_2^2)^{\frac{1}{2}}]^{-k} C_k^{\ell+1}(a_1/[a_1^2+c_1^2]^{\frac{1}{2}}) C_k^{\ell+1}(a_2/[a_2^2+c_2^2]^{\frac{1}{2}}) \quad (5.3.11)
\end{aligned}$$

Obviously, to generalize the previous results to the relativistic case we must calculate

$$\begin{aligned}
& \bar{K}_{\mu_1 \mu_2}^{\lambda \ell_1 \ell_2}(p_1, p_2; k_1, k_2; \omega) \\
&= \int_0^\infty r_1^{\mu_1} e^{-p_1 r_1 \omega} j_{\ell_1}(k_1 r_1 \omega) h(r_1, r_2; \lambda, \omega) j_{\ell_2}(k_2 r_2 \omega) e^{-k_2 r_2 \omega} r_2^{\mu_2} dr_1 dr_2 \quad (5.3.12)
\end{aligned}$$

This integral will also allow for the calculation of slightly more general DLT's for the nonrelativistic Green function than that given by (5.3.1).

We begin by considering the Sturmian form of  $h$ , (4.3.3). On interchanging the integrals and the summation we find

$$\begin{aligned}
& \bar{K}_{\mu_1 \mu_2}^{\lambda \ell_1 \ell_2}(p_1, p_2; k_1, k_2; \omega) \\
&= (2\omega)^{\lambda+1} \sum_{k=0}^{\infty} \frac{k! / (k+1+\lambda-\nu)}{\Gamma(2\lambda+2+k)} I_{k\mu_1}^{\lambda \ell_1}(p_1; k; \omega) I_{k\mu_2}^{\lambda \ell_2}(p_2; k; \omega) \quad (5.3.13)
\end{aligned}$$

where

$$I_{n\mu}^{\lambda\ell}(p; k; \omega) = \int_0^\infty r^{\mu+\lambda} e^{-(p+1)r\omega} j_\ell(kr\omega) L_n^{2\lambda+1}(2r\omega) dr. \quad (5.3.14)$$

The integral can be performed in several ways. I have presented one solution in Appendix B.3. We can expand the Laguerre polynomial so that

$$\begin{aligned} I_{n\mu}^{\lambda\ell}(p; k; \omega) &= (2\omega)^{-\lambda-\mu-1} 1/n! \sum_{m=0}^n \begin{bmatrix} n \\ m \end{bmatrix} \frac{\Gamma(2\lambda+2+n)}{\Gamma(2\lambda+2+m)} (-1)^m \\ &\quad \times \int_0^\infty x^{m+\mu+\lambda} e^{-(p+1)x/2} j_\ell(kx/2) dx \\ &= 2^{-\ell} \omega^{-\lambda-\mu-1} k^{-\ell-1} [(p+1)^2+k^2]^{\frac{1}{2}(\ell-\mu-\lambda)} \\ &\quad \times \sum_{i=0}^{\ell} \begin{bmatrix} \ell \\ i \end{bmatrix} (-1)^i \sum_{m=0}^n \begin{bmatrix} n \\ m \end{bmatrix} \frac{\Gamma(2\lambda+2+n) \Gamma(m+\mu+\lambda+\ell+1) \Gamma(m+\mu+\lambda-\ell+i)}{n! \Gamma(2\lambda+2+m) \Gamma(m+\mu+\lambda+1+i)} \\ &\quad \times \left[ \frac{-2}{\sqrt{(p+1)^2+k^2}} \right]^m \sin(\theta[m+\mu+\lambda-\ell+2i]) \end{aligned} \quad (5.3.15)$$

#### 5.4 : INVERTING THE VARIABLES IN THE DOUBLE LAPLACE TRANSFORM OF $g_\ell$

I have already presented an interesting integral equation satisfied by  $g_\ell(r_1, r_2; \nu)$  (eqn. (3.3.2)). From this it is possible to derive an algebraic relationship between a DLT,  $K_{n_1 n_2}^\ell(p_1, p_2; \nu)$ , and related DLT's with the transform variables inverted. In the special case where  $n_1 \geq \ell$  and  $n_2 \geq \ell$  this reduces to an algebraic relationship between different DLT's of  $g_\ell$  involving only finite sums. We begin by considering this latter case.

We note that

$$\int_0^\infty x^{n+\nu/2} e^{-\alpha x} J_\nu(2\beta\sqrt{x}) dx = n! \beta^\nu e^{-\beta^2/\alpha} / \alpha^{n+\nu+1} L_n^\nu(\beta^2/\alpha) \quad (5.4.1)$$

for  $n+\nu > -1$ . Then, taking into account the integral equation for  $g_\ell$  (3.3.2)

$$\begin{aligned} 2m/\hbar^2 K_{n_1+\ell+1, n_2+\ell+1}^\ell(p_1, p_2; \nu) &= \\ &= \int_0^\infty r_1^{n_1+(2\ell+1)/2} r_2^{n_2+(2\ell+1)/2} e^{-(p_1 r_1 + p_2 r_2)/a\nu} \sqrt{r_1 r_2} g_\ell(r_1, r_2; \nu) dr_1 dr_2 \\ &= 1/(a\nu)^2 \int_0^\infty \sqrt{s_1 s_2} g_\ell(s_1, s_2; \nu) \int_0^\infty r_1^{n_1+(2\ell+1)/2} e^{-p_1 r_1/a\nu} J_{2\ell+1}\left[\frac{2\sqrt{r_1 s_1}}{a\nu}\right] dr_1 \\ &\quad \times \int_0^\infty r_2^{n_2+(2\ell+1)/2} e^{-p_2 r_2/a\nu} J_{2\ell+1}\left[\frac{2\sqrt{r_2 s_2}}{a\nu}\right] dr_2 ds_1 ds_2, \end{aligned}$$

$$\begin{aligned}
&= n_1! n_2! (a\nu)^{n_1+n_2} p_1^{-n_1-2\ell-2} p_2^{-n_2-2\ell-2} \int_0^\infty (s_1 s_2)^{\ell+1} e^{-(s_1/p_1 + s_2/p_2)/a\nu} \\
&\quad \times L_{n_1}^{2\ell+1} \left[ \frac{s_1}{p_1 a\nu} \right] L_{n_2}^{2\ell+1} \left[ \frac{s_2}{p_2 a\nu} \right] g(s_1, s_2; \nu) ds_1 ds_2. \quad (5.4.2)
\end{aligned}$$

This last expression is just a finite sum of DLT's with the variables inverted. Thus

$$\begin{aligned}
K_{n_1+\ell+1, n_2+\ell+1}^\ell(p_1, p_2; \nu) &= (a\nu)^{n_1+n_2} p_1^{-n_1-2\ell-2} p_2^{-n_2-2\ell-2} \\
&\times \sum_{m_1=0}^{n_1} \left[ \begin{matrix} n_1 \\ m_1 \end{matrix} \right] \frac{(n_1+2\ell+1)!}{(m_1+2\ell+1)!} (-p_1 a\nu)^{-m_1} \sum_{m_2=0}^{n_2} \left[ \begin{matrix} n_2 \\ m_2 \end{matrix} \right] \frac{(n_2+2\ell+1)!}{(m_2+2\ell+1)!} (-p_2 a\nu)^{-m_2} \\
&\times K_{m_1+\ell+1, m_2+\ell+1}^\ell(1/p_1, 1/p_2; \nu). \quad (5.4.3)
\end{aligned}$$

Suppose  $n_1=n_2=0$ ; then (5.4.3) states that

$$p_1^{2\ell+2} p_2^{2\ell+2} K_{\ell+1, \ell+1}^\ell(p_1, p_2; \nu) = K_{\ell+1, \ell+1}^\ell(1/p_1, 1/p_2; \nu) \quad (5.4.4)$$

which is easily checked given (5.1.2).

We can do a similar calculation for general  $n_1$  and  $n_2$ . The expression will not now in general involve a finite sum of DLT's. The general form of (5.4.1) is

$$\begin{aligned}
&\int_0^\infty x^{\mu-1/2} e^{-\alpha x} J_{2\nu}(2\beta\sqrt{x}) dx = \\
&\frac{\Gamma(\mu+\nu+1/2)}{\Gamma(2\nu+1)} \beta^{2\nu} \alpha^{-\mu-\nu-1/2} {}_1F_1(\nu+\mu+1/2; 2\nu+1; -\beta^2/\alpha) \quad (5.4.5)
\end{aligned}$$

and, using the same reasoning as before we can show

$$\begin{aligned}
K_{n_1 n_2}^{\ell}(p_1, p_2; \nu) &= (n_1 + \ell)!(n_2 + \ell)!(a\nu)^{n_1 + n_2 - 2\ell - 2} p_1^{-n_1 - \ell - 1} p_2^{-n_2 - \ell - 1} \\
&\times \sum_{m_1=0}^{\infty} \frac{(\ell - n_1 + m_1)!}{(\ell - n_1)!(2\ell + 1 + m_1)!m_1!} (p_1 a\nu)^{-m_1} \sum_{m_2=0}^{\infty} \frac{(\ell - n_2 + m_2)!}{(\ell - n_2)!(2\ell + 1 + m_2)!m_2!} (p_2 a\nu)^{-m_2} \\
&\times K_{m_1 + \ell + 1, m_2 + \ell + 1}^{\ell}(1/p_1, 1/p_2; \nu) \quad (5.4.6)
\end{aligned}$$

These two transformation formulae, (5.4.3) and (5.4.6) can be thought of as analytic continuation formulae for the DLT's since they allow for the calculation of the DLT's in regions where the given formulae may not be convergent.

## CHAPTER 6 : THE REDUCED COULOMB GREEN FUNCTIONS

### 6.1 : THE REDUCED SCHRODINGER-COULOMB GREEN FUNCTION

The reduced Schrodinger-Coulomb Green function,  $\hat{G}(\mathbf{r}_1, \mathbf{r}_2; n)$  corresponding to the energy  $E_n$  is defined to be the solution of

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 - \frac{\hbar^2}{amr_1} - E_n \right] \hat{G}(\mathbf{r}_1, \mathbf{r}_2; n) = \delta(\mathbf{r}_1 - \mathbf{r}_2) - \sum \psi_n(\mathbf{r}_1) \psi_n^*(\mathbf{r}_2) \quad (6.1.1)$$

where the sum is over the entire manifold of states with energy  $E_n$ .

We now follow the same steps we used in solving the full Schrodinger-Coulomb Green function. We begin by expanding  $\hat{G}$  in terms of spherical harmonics,

$$\hat{G}(\mathbf{r}_1, \mathbf{r}_2; n) = \sum_{\ell m} \hat{g}_{\ell}(r_1, r_2; n) Y_{\ell m}(\theta_1, \phi_1) Y_{\ell m}^*(\theta_2, \phi_2) \quad (6.1.2)$$

and substitute this expansion into (6.1.1). Since there is a restriction on the maximum value of  $\ell$  possible in the manifold of states with principal quantum number  $n$ , there are two radial equations for  $\hat{g}$  :

$$\left[ \frac{1}{r_1} \frac{d}{dr_1} \left[ r_1^2 \frac{d}{dr_1} \right] - \frac{\ell(\ell+1)}{r_1^2} + \frac{2}{ar_1} - \frac{1}{a^2 n^2} \right] \hat{g}_{\ell}(r_1, r_2; n) = - (2m/\hbar^2) \frac{\delta(r_1 - r_2)}{r_1 r_2} \quad \text{for } \ell \geq n \quad (6.1.3a)$$

$$= - (2m/\hbar^2) \left[ \frac{\delta(r_1 - r_2)}{r_1 r_2} - R_{n\ell}(r_1) R_{n\ell}(r_2) \right] \quad \text{for } \ell < n \quad (6.1.3b)$$



It is immediately clear that for  $\ell \geq n$  the reduced radial functions are identical to the full radial functions obtained in Chapter 3,

$$\hat{g}_\ell(r_1, r_2; n) = g_\ell(r_1, r_2; n) \quad \text{for } \ell \geq n. \quad (6.1.4)$$

The solution of the second equation requires first a discussion of the appropriate boundary conditions.

Consideration of the forms of the full radial Green function and the radial wavefunctions leads us to require initially that

$$\hat{g}_\ell(r_1, r_2; n) \rightarrow O(r_1^\ell) \quad \text{as } r_1 \rightarrow 0, \quad (6.1.5a)$$

$$\hat{g}_\ell(r_1, r_2; n) \rightarrow e^{-r_1/a_n} \quad \text{as } r_1 \rightarrow \infty, \quad (6.1.5b)$$

$$\text{and } \hat{g}_\ell(r_1, r_2; n) = \hat{g}_\ell(r_2, r_1; n). \quad (6.1.5c)$$

We further require that  $\hat{g}_\ell$  be unique. It follows from the general definition of the reduced Green functions that they must be orthogonal to the relevant energy eigenspace. Since adding terms in  $R_{n\ell}$  to  $\hat{g}_\ell$  will not effect (6.1.3b) we make the following additional restriction on  $\hat{g}_\ell$ :

$$\int_0^\infty R_{n\ell}(r_1) \hat{g}_\ell(r_1, r_2; n) r_1^2 dr_1 = 0, \quad (6.1.6)$$

and similarly for  $r_2$ . These formalities over we can now quite rapidly solve equation (6.1.3b).

We begin by reminding ourselves of the expansion of the  $\delta$ -function in terms of Laguerre polynomials, equation (3.1.20), and also of the action

of the radial hamiltonian on eigenstate-type functions, equation (2.3.28).

We are then led to a trial solution of (6.1.3b) of the form

$$g(r_1, r_2) = (2/an)^{2\ell+1} (r_1 r_2)^\ell e^{-(r_1+r_2)/an} \times \left[ \sum_{k=0}^{\infty *} \frac{k!}{(2\ell+1+k)!(\ell+1+k-n)} L_k^{2\ell+1}(2r_1/an) L_k^{2\ell+1}(2r_2/an) + \sum_{i=0}^{\infty} \alpha_i L_i^{2\ell+1}(2r_1/an) L_{n-\ell-1}^{2\ell+1}(2r_2/an) \right] \quad (6.1.7)$$

where the asterix indicates that we omit the term  $k=n-\ell-1$  from the summation and the  $\alpha_i$  are constants to be determined from the boundary conditions. Then, inserting this trial function into the LHS of (6.1.3b), and using (3.1.20) and (2.3.28) gives us

$$\begin{aligned} & \left[ \frac{d^2}{dr_1^2} + \frac{2}{r_1} \frac{d}{dr_1} - \frac{\ell(\ell+1)}{r_1^2} + \frac{2}{ar_1} + \frac{1}{a^2 n^2} \right] g(r_1, r_2) = -(2/an)^{2\ell+2} r_1^{\ell-1} r_2^\ell \\ & \times e^{-(r_1+r_2)/an} \left[ \sum_{k=0}^{\infty *} \frac{k!}{(2\ell+1+k)!} L_k^{2\ell+1}(2r_1/an) L_k^{2\ell+1}(2r_2/an) \right. \\ & \quad \left. + \sum_{i=0}^{\infty} \alpha_i (\ell+1+i-n) L_i^{2\ell+1}(2r_1/an) L_{n-\ell-1}^{2\ell+1}(2r_2/an) \right] \\ & = - \frac{\delta(r_1-r_2)}{r_1 r_2} + \\ & (2/an)^{2\ell+2} r_1^{\ell-1} r_2^\ell e^{-(r_1+r_2)/an} \left[ \frac{(n-\ell-1)!}{(n+\ell)!} L_{n-\ell-1}^{2\ell+1}(2r_1/an) L_{n-\ell-1}^{2\ell+1}(2r_2/an) \right. \\ & \quad \left. - \sum_{i=0}^{\infty} \alpha_i (\ell+1+i-n) L_i^{2\ell+1}(2r_1/an) L_{n-\ell-1}^{2\ell+1}(2r_2/an) \right] \quad (6.1.8) \end{aligned}$$

Comparing this last expression with the RHS of (6.1.3b) and noting the form of  $R_{n\ell}$  given in Chapter 2, we see that we must choose the  $\alpha_i$ 's such

that

$$\begin{aligned} \sum_{i=0}^{\infty} \alpha_i (\ell+1+i-n) L_i^{2\ell+1}(2r_1/an) &= \frac{(n-\ell-1)!}{2n(n+\ell)!} (2n-2r_1/an) L_{n-\ell-1}^{2\ell+1}(2r_1/an) \\ &= \frac{(n-\ell-1)!}{2n(n+\ell)!} \left[ (n-\ell) L_{n-\ell}^{2\ell+1}(2r_1/an) + (n+\ell) L_{n-\ell-2}^{2\ell+1}(2r_1/an) \right] \end{aligned} \quad (6.1.9)$$

where, in the last step we have used a standard recursion relation of Laguerre polynomials (see Appendix A.1). As we might have expected from the above remarks on the boundary conditions,  $\alpha_{n-\ell-1}$  is not determined by (6.1.9). However, given that the Laguerre polynomials (with an appropriate weight function) are an orthonormal set we deduce that

$$\alpha_{n-\ell} = \frac{(n-\ell)!}{2n(n+\ell)!}, \quad \alpha_{n-\ell-2} = -\frac{(n-\ell-1)!}{2n(n+\ell-1)!}, \quad (6.1.10)$$

and all other  $\alpha_i$  with the possible exception of  $\alpha_{n-\ell-1}$  are zero. As the final step in our solution of (6.1.3b) we note that we may add to  $g$  any multiple of  $L_{n-\ell-1}^{2\ell+1}(2r_1/an)$  we desire in order to make the solution symmetrical (eqn. (6.1.5c)) and to make it satisfy the orthogonality condition (6.1.6). We note here the relation

$$\begin{aligned} \int_0^{\infty} \sigma^{2\ell+2} e^{-\sigma} L_i^{2\ell+1}(\sigma) L_j^{2\ell+1}(\sigma) d\sigma &= \frac{(2\ell+2+i)!}{i!} [\delta_{j,i} - \delta_{j,i+1}] \\ &+ \frac{(2\ell+1+i)!}{(i-1)!} [\delta_{j,i} - \delta_{j,i-1}] \end{aligned} \quad (6.1.11)$$

which is useful in discovering the correct combinations to satisfy this final condition. The full solution is then found to be

$$\begin{aligned}
\hat{g}_\ell(r_1, r_2; n) &= (2/an)^{2\ell+1} (r_1 r_2)^\ell e^{-(r_1+r_2)/an} \\
&\times \left[ \sum_{k=0}^{\infty} \frac{k!}{(2\ell+1+k)!(\ell+1+k-n)} L_k^{2\ell+1}(2r_1/an) L_k^{2\ell+1}(2r_2/an) \right. \\
&+ \frac{(n-\ell-1)!}{2n(n+\ell)!} \left[ L_{n-\ell-1}^{2\ell+1}(2r_1/an) \left[ (n-\ell)L_{n-\ell}^{2\ell+1}(2r_2/an) - (n+\ell)L_{n-\ell-2}^{2\ell+1}(2r_2/an) \right] \right. \\
&\quad \left. + L_{n-\ell-1}^{2\ell+1}(2r_1/an) L_{n-\ell-1}^{2\ell+1}(2r_2/an) \right. \\
&\quad \left. + \left[ (n-\ell)L_{n-\ell}^{2\ell+1}(2r_1/an) - (n+\ell)L_{n-\ell-2}^{2\ell+1}(2r_1/an) \right] L_{n-\ell-1}^{2\ell+1}(2r_2/an) \right] \Bigg\}
\end{aligned}
\tag{6.1.12}$$

## 6.2 : THE DOUBLE LAPLACE TRANSFORM OF THE REDUCED SCHRÖDINGER-COULOMB GREEN FUNCTION

The double Laplace transforms of finite sums of Laguerre polynomials in the Sturmian expansion for  $\hat{g}_\ell$  pose no real difficulty. We must, however, find some way of dealing with at least part of the infinite sum. This we do now. Omitting the first  $n-\ell-2$  terms in the infinite sum (6.1.12) let us calculate the double Laplace transform of

$$\begin{aligned} \hat{g}_\ell^*(r_1, r_2; n) &= (r_1 r_2)^\ell e^{-(r_1+r_2)/an} \\ &\times \sum_{k=n-\ell}^{\infty} \frac{k!}{(2\ell+1+k)!(\ell+1+k-n)} L_k^{2\ell+1}(2r_1/an) L_k^{2\ell+1}(2r_2/an). \end{aligned} \quad (6.2.1)$$

Then,

$$\begin{aligned} K_{\ell+1, \ell+1}^{\ell}(p_1, p_2; n) &= \int_0^\infty (r_1 r_2)^{\ell+1} \hat{g}_\ell^*(r_1, r_2; n) e^{-(p_1 r_1 + p_2 r_2)/an} dr_1 dr_2 \\ &= \sum_{k=n-\ell}^{\infty} \frac{k!}{(2\ell+1+k)!(\ell+1+k-n)} \int_0^\infty r_1^{2\ell+1} e^{-(p_1+1)r_1/an} L_k^{2\ell+1}(2r_1/an) dr_1 \\ &\quad \times \int_0^\infty r_2^{2\ell+1} e^{-(p_2+1)r_2/an} L_k^{2\ell+1}(2r_2/an) dr_2 \\ &= (an)^{4\ell+4} [(p_1+1)(p_2+1)]^{-2\ell-2} \sum_{k=n-\ell}^{\infty} \frac{(2\ell+1+k)!}{k!(\ell+1+k-n)} \left[ \frac{p_1-1}{p_1+1} \right]^k \left[ \frac{p_2-1}{p_2+1} \right]^k. \end{aligned} \quad (6.2.2)$$

I have calculated this last sum in Appendix B.5. Thus, using (B.5.3) one finds that

$$\begin{aligned}
K_{\ell+1,\ell+1}^{*\ell}(p_1,p_2;n) &= (an)^{4\ell+4}[(p_1+1)(p_2+1)]^{-2\ell-2} \left[\frac{p_1-1}{p_1+1}\right]^{n-\ell-1} \left[\frac{p_2-1}{p_2+1}\right]^{n-\ell-1} \\
&\times \left\{ (2\ell+1)! \sum_{k=0}^{2\ell} \frac{(n-\ell-1+k)!(-1)^k}{k!(n-\ell-1)!(k-2\ell-1)} \left[\frac{(p_1+1)(p_2+1)}{-2(p_1+p_2)}\right]^{2\ell+1-k} \right. \\
&\quad \left. \frac{(n+\ell)!}{(n-\ell-1)!} \log \left[\frac{2(p_1+p_2)}{(p_1+1)(p_2+1)}\right] \right\}. \quad (6.2.3)
\end{aligned}$$

The double Laplace transforms of the Laguerre polynomials can be performed using (3.1.18). We thus arrive at the following form of the DLT of the reduced Schrodinger-Coulomb Green function:

$$\begin{aligned}
\tilde{K}_{\ell+1,\ell+1}^{\ell}(p_1,p_2;n) &= (2/an)^{2\ell+1} K_{\ell+1,\ell+1}^{*\ell}(p_1,p_2;n) + (2)^{2\ell+1}(an)^{2\ell+3} \\
&\times \left[ [(p_1+1)(p_2+1)]^{-2\ell-2} \sum_{k=0}^{n-\ell-2} \frac{(2\ell+1+k)!}{(\ell+1+k-n)k!} \left[\frac{p_1-1}{p_1+1}\right]^k \left[\frac{p_2-1}{p_2+1}\right]^k \right. \\
&\quad \left. + \frac{2}{n} \left[\frac{p_1-1}{p_1+1}\right]^n \left[\frac{p_2-1}{p_2+1}\right]^n [(p_1-1)(p_2-1)]^{-\ell-2} (p_1p_2-1)[(\ell+1)(p_1p_2+1)-n(p_1+p_2)] \right]. \quad (6.2.4)
\end{aligned}$$

Johnson<sup>26</sup> has remarked that the Sturmian form of the reduced Coulomb Green function is unsuitable for the calculation of matrix elements. I hope to have shown that very simple manipulations can lead to quite convenient forms, similar to those calculated by Hill and Huxtable<sup>13</sup>.

## CHAPTER 7: TWO PHOTON BOUND STATE -- BOUND STATE TRANSITIONS IN ATOMIC HYDROGEN.

### 7.0 : INTRODUCTION

In the previous chapters I have presented a comprehensive overview of the Coulomb Green functions and their matrix elements. As I indicated in Chapter 1, this theory may be applied to many different physical phenomena related to the quantum theory of the hydrogen atom involving specifically the interaction of the electron with more than one photon. Probably the most straightforward of these phenomena is the transition between two bound states accompanied by the emission of two photons; the most widely studied of these processes is the two photon decay of the  $2s_{1/2}$  level to the ground state.

The selection rules for single photon transitions show that the  $2s_{1/2}$  level of hydrogenic ions is stable to single photon electric dipole transitions. Although single photon magnetic dipole transitions are allowed, the dominant decay mechanism is now known to be by the simultaneous emission of two electric dipole photons. Estimates of the lifetime of the  $2s_{1/2}$  state were first made by Breit and Teller<sup>48</sup> in 1940, and later by others who performed their calculation of the two photon transition rate by summing the various terms involving intermediate states (see below) term by term. Somewhat later calculations making use of the Green function formalism were made by Rapoport and Zon<sup>49</sup>, and by Klarsfeld<sup>50</sup> in the nonrelativistic dipole approximation. Relativistic calculations including retardation have since been performed by Goldman and Drake<sup>3</sup> using a variationally determined finite basis set.

In the next section I will present the theory of two photon transitions in the relativistic formulation of quantum electrodynamics as it relates to the theory of the Coulomb Green functions. I will omit the quantum electrodynamical part of the theory which is quite standard and can be found in many texts, and I will begin with the basic expression for the differential emission rate. In the final section I present a nonrelativistic calculation of the E1E1 decay rate of the  $2s_{\frac{1}{2}}$  level without making the long wavelength approximation as a demonstration of the utility of employing general methods to the solution of two photon problems.

## 7.2 : THE THEORY OF TWO PHOTON TRANSITIONS.

The relativistic differential emission rate for two photons of energy  $\omega_j$  and polarization direction  $\hat{\epsilon}_j$  emitted into the solid angle  $d\Omega_j$  from the initial state  $i$  to the final state  $f$  is given by

$$\frac{dw}{d\omega_1} = (\alpha^2/(2\pi)^2) (\hbar^2/m^4 c^4) \omega_1 \omega_2 |M|^2 d\Omega_1 d\Omega_2 \quad (7.2.1)$$

with

$$\begin{aligned} M = & \langle f | \hat{\alpha}_1 \hat{\epsilon}_2 e^{-i\vec{k}_2 \cdot \vec{r}} G(E_i - \hbar\omega_1) \hat{\alpha} \cdot \hat{\epsilon}_1 e^{-i\vec{k}_1 \cdot \vec{r}} | i \rangle \\ & + \langle f | \hat{\alpha} \cdot \hat{\epsilon}_1 e^{-i\vec{k}_1 \cdot \vec{r}} G(E_i - \hbar\omega_2) \hat{\alpha}_1 \hat{\epsilon}_2 e^{-i\vec{k}_2 \cdot \vec{r}} | i \rangle \end{aligned} \quad (7.2.2)$$

and where  $|\vec{k}_j| = \omega_j / c$ .

It is possible to separate the dependence on the angular parts of  $\vec{k}_1$  and  $\vec{k}_2$  from the rest of the preceding expression. This is accomplished by



writing

$$e^{-i\mathbf{k} \cdot \mathbf{r}} = \sum_{\ell m \lambda} [r \cdot \vec{Y}_{\ell m}^{\lambda}(\Omega)] a_{\ell m}^{\lambda}(\mathbf{r}, k)^* \quad (7.2.3)$$

where the  $\vec{Y}_{\ell m}^{\lambda}$ 's are related to the usual vector spherical harmonics by

$$\vec{Y}_{\ell m}^{+1} = \sqrt{\ell/(2\ell+1)} \vec{Y}_{\ell\ell+1m} + \sqrt{(\ell+1)/(2\ell+1)} \vec{Y}_{\ell\ell-1m}, \quad (7.2.4a)$$

$$\vec{Y}_{\ell m}^0 = \vec{Y}_{\ell\ell m}, \quad (7.2.4b)$$

$$\vec{Y}_{\ell m}^{-1} = -\sqrt{(\ell+1)/(2\ell+1)} \vec{Y}_{\ell\ell+1m} + \sqrt{\ell/(2\ell+1)} \vec{Y}_{\ell\ell-1m}, \quad (7.2.4c)$$

and

$$a_{\ell m}^{+1}(\mathbf{r}, k) = \sqrt{\ell/(2\ell+1)} g_{\ell+1}(kr) \vec{Y}_{\ell\ell+1m}(\Omega) + \sqrt{(\ell+1)/(2\ell+1)} g_{\ell-1}(kr) \vec{Y}_{\ell\ell-1m}(\Omega), \quad (7.2.5a)$$

$$a_{\ell m}^0(\mathbf{r}, k) = g_{\ell}(kr), \quad (7.2.5b)$$

$$a_{\ell m}^{-1}(\mathbf{r}, k) = \sqrt{\ell/(2\ell+1)} g_{\ell-1}(kr) \vec{Y}_{\ell\ell-1m}(\Omega) - \sqrt{(\ell+1)/(2\ell+1)} \vec{Y}_{\ell\ell+1m}(\Omega); \quad (7.2.5c)$$

with  $g_{\ell}(x) = 4\pi i^{\ell} j_{\ell}(x)$  proportional to the spherical Bessel function.

The term within the modulus sign in equation (7.2.1) thus becomes

$$\begin{aligned}
M = \sum_{\ell m \lambda} & [\hat{\epsilon}_1 \cdot \hat{Y}_{\ell_1 m_1}^{\lambda_1}(\Omega_1)] [\hat{\epsilon}_2 \cdot \hat{Y}_{\ell_2 m_2}^{\lambda_2}(\Omega_2)] \\
& \times \left[ \langle f | \hat{\alpha} \cdot \hat{a}_{\ell_2 m_2}^{\lambda_2}(k_2)^* G(E_i - \hbar\omega_1) \hat{\alpha} \cdot \hat{a}_{\ell_1 m_1}^{\lambda_1}(k_1)^* | i \rangle \right. \\
& \left. + \langle f | \hat{\alpha} \cdot \hat{a}_{\ell_1 m_1}^{\lambda_1}(k_1)^* G(E_i - \hbar\omega_2) \hat{\alpha} \cdot \hat{a}_{\ell_2 m_2}^{\lambda_2}(k_2)^* | i \rangle \right], \quad (7.2.6)
\end{aligned}$$

where the sum is over both indices. Electric (EL) type transitions correspond to  $\lambda=+1$ , magnetic (ML) transitions to  $\lambda=0$ . We need not consider the case when  $\lambda=-1$  since those terms vanish in the Coulomb gauge. Adopting the notation of Goldman and Drake<sup>3</sup>, we see that

$$\begin{aligned}
|M|^2 = \sum_{\ell m \lambda} & C_{\ell_1 m_1 \lambda_1}^{\ell m \lambda} C_{\ell_2 m_2 \lambda_2}^{\ell m \lambda} \\
& \times (B_{\ell_1 m_1 \lambda_1}^{\ell_2 m_2 \lambda_2} + B_{\ell_2 m_2 \lambda_2}^{\ell_1 m_1 \lambda_1}) (B_{\ell_1 m_1 \lambda_1}^{\ell_2 m_2 \lambda_2} + B_{\ell_2 m_2 \lambda_2}^{\ell_1 m_1 \lambda_1})^* \quad (7.2.7)
\end{aligned}$$

with

$$C_{\ell m \lambda}^{\ell' m' \lambda'} = [\hat{\epsilon} \cdot \hat{Y}_{\ell m}^{\lambda}] [\hat{\epsilon}' \cdot \hat{Y}_{\ell' m'}^{\lambda'}]^*, \quad (7.2.8)$$

$$B_{\ell_1 m_1 \lambda_1}^{\ell_2 m_2 \lambda_2} = \langle f | \hat{\alpha} \cdot \hat{a}_{\ell_2 m_2}^{\lambda_2}(k_2)^* G(E_i - \hbar\omega_1) \hat{\alpha} \cdot \hat{a}_{\ell_1 m_1}^{\lambda_1}(k_1)^* | i \rangle. \quad (7.2.9)$$

Now,

$$\int \Sigma_{\hat{\epsilon}} C_{\ell m \lambda}^{\ell' m' \lambda'} d\Omega = \delta_{\ell \ell'} \delta_{m m'} \delta_{\lambda \lambda'}, \quad (7.2.10)$$

which allows us to write the differential emission rate, integrated over angles and summed over the possible polarization directions as

$$\frac{dW}{d\omega_1} = \omega_1 \omega_2 \sum_{\substack{\ell_1 m_1 \lambda_1 \\ \ell_2 m_2 \lambda_2}} | B_{\ell_1 m_1 \lambda_1}^{\ell_2 m_2 \lambda_2} + B_{\ell_2 m_2 \lambda_2}^{\ell_1 m_1 \lambda_1} |^2 \quad (7.2.11)$$

We now perform the angular integrals implicit in  $B$ . We follow the method due to Grant<sup>51</sup>, adapted to our Green function formulation. We begin by noting the expansion of  $G$  in terms of spinor spherical harmonics given by (4.1.2), and by writing

$$\langle \uparrow | i \rangle = \begin{bmatrix} f_{11}(r) \chi_{\kappa_1}^{M_1} \\ i f_{21}(r) \chi_{-\kappa_1}^{M_1} \end{bmatrix}, \quad \langle \uparrow | f \rangle = \begin{bmatrix} f_{12}(r) \chi_{\kappa_2}^{M_2} \\ i f_{22}(r) \chi_{-\kappa_2}^{M_2} \end{bmatrix}, \quad (7.2.12)$$

and

$$\partial \cdot \partial_{\ell m}^{\lambda(k)*} = \begin{bmatrix} 0 & \partial \cdot \partial \\ \partial \cdot \partial & 0 \end{bmatrix} \quad (7.2.13)$$

so that

$$\begin{aligned} & \partial \cdot \partial_{\ell_2 m_2}^{\lambda_2(k_2)*} G(E_i - \hbar \omega_1) \partial \cdot \partial_{\ell_1 m_1}^{\lambda_1(k_1)*} \\ &= \sum_{\kappa \mu} \begin{bmatrix} g_{\kappa}^{22} \partial \cdot \partial_2 \chi_{-\kappa}^{\mu} \chi_{-\kappa}^{\mu\dagger} \partial \cdot \partial_1 & i g_{\kappa}^{21} \partial \cdot \partial_2 \chi_{-\kappa}^{\mu} \chi_{\kappa}^{\mu\dagger} \partial \cdot \partial_1 \\ i g_{\kappa}^{12} \partial \cdot \partial_2 \chi_{\kappa}^{\mu} \chi_{-\kappa}^{\mu\dagger} \partial \cdot \partial_1 & g_{\kappa}^{11} \partial \cdot \partial_2 \chi_{\kappa}^{\mu} \chi_{\kappa}^{\mu\dagger} \partial \cdot \partial_1 \end{bmatrix} \end{aligned} \quad (7.2.14)$$

where the notational contractions should be self explanatory. Thus, defining

$$\chi_{2\kappa\mu}^{\pm\pm} = \chi_{\pm\kappa_2}^{M_2\dagger} \partial \cdot \partial_2 \chi_{\pm\kappa}^{\mu}, \quad \chi_{1\kappa\mu}^{\pm\pm} = \chi_{\pm\kappa}^{\mu\dagger} \partial \cdot \partial_1 \chi_{\pm\kappa_1}^{M_1} \quad (7.2.15)$$

we find

$$B_{\ell_1 m_1 \lambda_1}^{\ell_2 m_2 \lambda_2} = \sum_{\kappa \mu} \int [ (f_{12} g_{\kappa} f_{11}) [\chi_{2\kappa\mu}^{+ -} \chi_{2\kappa\mu}^{- +}] - (f_{12} g_{\kappa} f_{21}) [\chi_{2\kappa\mu}^{+ -} \chi_{1\kappa\mu}^{+ -}] + (f_{22} g_{\kappa} f_{11}) [\chi_{2\kappa\mu}^{- +} \chi_{1\kappa\mu}^{- +}] + (f_{22} g_{\kappa} f_{21}) [\chi_{2\kappa\mu}^{- +} \chi_{1\kappa\mu}^{+ -}] ] d\tau_1 d\tau_2 . \quad (7.2.16)$$

Examination of the nature of the  $\chi$ 's introduced above shows that the angular integrals can be performed once we know how to calculate

$$I_{\kappa\mu\kappa'\mu'}^{L\lambda M} = \int \chi_{\kappa}^{\mu\dagger} \partial \cdot \vec{Y}_{LL+\lambda M} \chi_{\kappa'}^{\mu'} d\Omega . \quad (7.2.17)$$

This integral has been calculated by Grant<sup>51</sup>. The procedure consists of recognizing that  $\partial \cdot \vec{Y}_{LL+\lambda M}$  is a coupled spherical tensor of rank  $L$  :

$$\partial \cdot \vec{Y}_{LL+\lambda M} = [\sigma \otimes Y^{L+\lambda}]_M^L \equiv X^{(\lambda)}_{LM} . \quad (7.2.18)$$

Then

$$I_{\kappa\mu\kappa'\mu'}^{L\lambda M} = \langle \ell, 1/2; j, \mu | X^{(\lambda)}_{LM} | \ell', 1/2; j', \mu' \rangle \quad (7.2.19)$$

where as usual, for example,  $\ell = |\kappa + 1/2| - 1/2$  and  $j = |\kappa| - 1/2$ . It is possible to employ the Wigner-Eckart theorem to write the matrix element in terms of the reduced matrix element of  $X$ , and to then express that in terms of the reduced matrix elements of  $\partial$  and  $Y^{L+\lambda}$ . Thus

$$I_{\kappa\mu\kappa'\mu'}^{L\lambda M} = (-1)^{j-\mu} \begin{bmatrix} j & L & j' \\ -\mu & M & \mu' \end{bmatrix} \langle \ell, 1/2; j || X^{(\lambda)}_L || \ell', 1/2; j' \rangle$$

$$\begin{aligned}
&= (-1)^{j-\mu} \begin{bmatrix} j & L & j' \\ -\mu & M & \mu' \end{bmatrix} [j, j', L]^{\frac{1}{2}} \begin{bmatrix} \ell & 1/2 & j \\ \ell' & 1/2 & j' \\ L+\lambda & 1 & L \end{bmatrix} \\
&\quad \times \langle \ell \| Y^{L+\lambda} \| \ell' \rangle \langle 1/2 \| \sigma \| 1/2 \rangle, \quad (7.2.20)
\end{aligned}$$

where we have introduced the notation  $[\ell, \ell', \dots] = (2\ell+1)(2\ell'+1)\dots$ , and where

$$\langle \ell \| Y^{L+\lambda} \| \ell' \rangle = (-1)^\ell [\ell, \ell', L+\lambda]^{\frac{1}{2}} / \sqrt{4\pi} \begin{bmatrix} \ell & L+\lambda & \ell' \\ 0 & 0 & 0 \end{bmatrix},$$

$$\langle 1/2 \| \sigma \| 1/2 \rangle = \sqrt{6}.$$

Now

$$\begin{aligned}
&\begin{bmatrix} \ell & \ell' & L+\lambda \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} j & j' & L \\ \ell & \ell' & L+\lambda \\ 1/2 & 1/2 & 1 \end{bmatrix} \\
&= \sum_{\substack{\mu \mu' m \\ s s' q}} \begin{bmatrix} j & j' & L \\ \mu & \mu' & m \end{bmatrix} \begin{bmatrix} 1/2 & 1/2 & 1 \\ s & s' & q \end{bmatrix} \begin{bmatrix} j & \ell & 1/2 \\ \mu & 0 & s \end{bmatrix} \begin{bmatrix} j' & \ell' & 1/2 \\ \mu' & 0 & s' \end{bmatrix} \begin{bmatrix} L & L+\lambda & 1 \\ m & 0 & q \end{bmatrix} \\
&\quad (7.2.21)
\end{aligned}$$

which is actually only a sum over  $s$  and  $s'$ ; thus there are at most only four terms in the expansion. It is a simple matter to compute the sums explicitly so that finally we have

$$I_{\kappa \mu \kappa' \mu'}^{L0M} = J_{\kappa \mu \kappa' \mu'}^{LM} \times (-1)^{j+\frac{1}{2}} (\kappa - \kappa') \sqrt{(2L+1)/L(L+1)} [1 + (-1)^{\ell+\ell'+L}]/2, \quad (7.2.22a)$$

$$I_{\kappa \mu \kappa' \mu'}^{L1M} = J_{\kappa \mu \kappa' \mu'}^{LM} \times (-1)^{j+\frac{1}{2}} (L+1+\kappa+\kappa') 1/\sqrt{L+1} [1 + (-1)^{\ell+\ell'+L+1}]/2, \quad (7.2.22b)$$

$$I_{\kappa \mu \kappa' \mu'}^{L-1M} = J_{\kappa \mu \kappa' \mu'}^{LM} \times (-1)^{j+\frac{1}{2}} (-L+\kappa+\kappa') 1/\sqrt{L} [1 + (-1)^{\ell+\ell'+L-1}]/2, \quad (7.2.22c)$$

where

$$J_{\kappa\mu\kappa'\mu'}^{LM} = (-1)^{j-\mu} \begin{bmatrix} j & L & j' \\ 1/2 & 0 & -1/2 \end{bmatrix} \begin{bmatrix} j & L & j' \\ -\mu & M & \mu' \end{bmatrix} [jj']^{1/2} / \sqrt{4\pi} \quad (7.2.23)$$

Since we are working in the Coulomb gauge it is only necessary to include the  $\lambda=0,1$  terms in our calculation. Thus;

$$\begin{aligned} I_{\kappa\mu\kappa'\mu'}^{LM(0)} &= \int \chi_{\kappa}^{\mu\dagger} \partial \cdot \vec{a}_{LM}^0 \chi_{\kappa'}^{\mu'} d\Omega \\ &= g_L I_{\kappa\mu\kappa'\mu'}^{L0M} ; \end{aligned} \quad (7.2.24)$$

$$\begin{aligned} I_{\kappa\mu\kappa'\mu'}^{LM(+1)} &= \int \chi_{\kappa}^{\mu\dagger} \partial \cdot \vec{a}_{LM}^{+1} \chi_{\kappa'}^{\mu'} d\Omega \\ &= \sqrt{L/2L+1} g_{L+1} I_{\kappa\mu\kappa'\mu'}^{L1M} + \sqrt{(L+1)/(2L+1)} g_{L-1} I_{\kappa\mu\kappa'\mu'}^{L-1M} \end{aligned} \quad (7.2.25)$$

(The corresponding equations in Goldman and Drake<sup>3</sup> seem to be missing the factors depending on  $\ell$  and  $\ell'$  which give rise to the parity selection rules.)

We have thus performed completely both angular integrations in  $B_{\ell_1 m_1 \lambda_1}^{\ell_2 m_2 \lambda_2}$ , and have remaining only integrals over  $r_1$  and  $r_2$  of the radial Dirac Coulomb Green function and spherical Bessel functions. It is a simple matter to express these integrals in terms of our transformed radial functions and thus calculate the resulting Double Laplace transforms. Nonetheless, there is still the summation over  $\kappa$  and  $\mu$  to contend with: it appears twice since  $B$  is squared in the expression for the transition rate (7.2.11).

Goldman and Drake<sup>3</sup> have shown that what is apparently a summation over four indices (two each for  $\kappa$  and  $\mu$ ) can be reduced to a

single summation over  $\kappa$ . Following them we separate out of  $B$  the factor dependent on  $\mu$ , that is we write

$$B_{\ell_1 m_1 \lambda_1}^{\ell_2 m_2 \lambda_2} = \sum_{\kappa} \bar{B}_{\ell_1 m_1 \lambda_1}^{\ell_2 m_2 \lambda_2(\kappa)} \times \theta^{\kappa}(2,1) \quad (7.2.26)$$

where

$$\theta^{\kappa}(2,1) = \sqrt{2j+1} \sum_{\mu} (-1)^{M_1+M_2+1} \begin{bmatrix} j_2 & \ell_2 & j \\ -M_2 & m_2 & \mu \end{bmatrix} \begin{bmatrix} j & \ell_1 & j_1 \\ -\mu & m_1 & M_1 \end{bmatrix} \quad (7.2.27)$$

and  $j = |\kappa| - 1/2$ .

The  $\theta$ 's satisfy two useful properties:

$$\sum_{m_1 m_2 M_1 M_2} \theta^{\kappa}(2,1) \theta^{\kappa'}(2,1) = \delta_{j,j'} ; \quad (7.2.28)$$

$$\sum_{m_1 m_2 M_1 M_2} \theta^{\kappa}(2,1) \theta^{\kappa'}(1,2) = [j,j']^{\frac{1}{2}} (-1)^{2j+\ell_1+\ell_2} \begin{bmatrix} j_2 & j & \ell_1 \\ j_1 & j & \ell_2 \end{bmatrix} . \quad (7.2.29)$$

Thus, the decay rate summed over  $m_1$  and averaged over  $m_2$  (at the same time summing over the magnetic quantum numbers of the multipole operators) is given by

$$\frac{dW}{d\omega_1} = \omega_1 \omega_2 / (2j+1) \sum_{\kappa} ( \sum_{\kappa} [ \theta^{\kappa}(2,1) \bar{B}_{\ell_1 m_1 \lambda_1}^{\ell_2 m_2 \lambda_2(\kappa)} + \theta^{\kappa}(1,2) \bar{B}_{\ell_2 m_2 \lambda_2}^{\ell_1 m_1 \lambda_1(\kappa)} ] )^2 \quad (7.2.30)$$

where the summation is over  $(\ell_1, \ell_2, m_1, m_2, \lambda_1, \lambda_2, M_1, M_2)$  which becomes

$$\begin{aligned}
\frac{d\bar{W}}{d\omega_1} = & \omega_1\omega_2/(2j_1+1) \sum_{\ell, \lambda} \left[ \bar{B}_{\ell_1 m_1 \lambda_1}^{\ell_2 m_2 \lambda_2}(\kappa)^2 + \bar{B}_{\ell_2 m_2 \lambda_2}^{\ell_1 m_1 \lambda_1}(\kappa)^2 \right. \\
& \left. + 2 \sum_{\kappa} (-1)^{2j'+\ell_1+\ell_2} [j, j']^{\frac{1}{2}} \begin{Bmatrix} j_2 & j' & \ell_1 \\ j_1 & j & \ell_2 \end{Bmatrix} \bar{B}_{\ell_1 m_1 \lambda_1}^{\ell_2 m_2 \lambda_2}(\kappa) \bar{B}_{\ell_2 m_2 \lambda_2}^{\ell_1 m_1 \lambda_1}(\kappa) \right] \quad (7.2.31)
\end{aligned}$$

This is then the basic expression for calculating two photon transition rates using the Green function methods.

It is important to note that the sum over  $\kappa$  in the final solution is not actually an infinite one; the allowed values of  $\kappa$  (ie.  $j$ ) are limited by the 3- $j$  symbol in equation (7.2.20). Further restrictions on the summations occur as a result of the parity selection rules implicit in the terms involving  $\ell$  and  $\ell'$  in equations (7.2.22)). A specific calculation will therefore start with the determination of the allowed intermediate states (ie.  $\kappa$ ) before the radial integrals are performed. For this reason I do not pursue the theory further here; rather than finding a completely general expression for the transition rates with explicitly evaluated integrals (which can be obtained from Chapter 5) I am content to calculate in the following section the nonrelativistic two photon transition rate for a very specific problem to illustrate the general method.



### 7.3 : THE NONRELATIVISTIC TWO PHOTON DECAY OF THE $2s_{\frac{1}{2}}$ LEVEL OF HYDROGENIC IONS.

The nonrelativistic two photon decay rate<sup>52</sup> (using the same notation as before) is given by

$$\frac{dW}{d\omega_1} = \alpha^2/(2\pi)^3 \hbar^2/m^4 c^4 \omega_1 \omega_2 |N|^2 d\Omega_1 d\Omega_2 \quad (7.3.1)$$

where

$$\begin{aligned} N = & \langle f | \vec{p} \cdot \vec{e}_2 e^{-i\vec{k}_2 \cdot \vec{r}} G(E_i - \hbar\omega_1) e^{-i\vec{k}_1 \cdot \vec{r}} \vec{e}_1 \cdot \vec{p} | i \rangle \\ & + \langle f | \vec{p} \cdot \vec{e}_1 e^{-i\vec{k}_1 \cdot \vec{r}} G(E_i - \hbar\omega_2) e^{-i\vec{k}_2 \cdot \vec{r}} \vec{e}_2 \cdot \vec{p} | i \rangle \\ & + m/2 \langle f | \vec{e}_1 \cdot \vec{e}_2 e^{-i(\vec{k}_1 + \vec{k}_2) \cdot \vec{r}} | i \rangle \end{aligned} \quad (7.3.2)$$

We treat  $\vec{e} e^{-i\vec{k} \cdot \vec{r}}$  in exactly the same manner as in the theory of relativistic two photon transitions given above. Then the decay rate integrated over photon wave vector angles and polarization directions becomes

$$\frac{d\dot{W}}{d\omega_1} = \alpha^2/(2\pi)^3 \hbar^2/m^4 c^4 \omega_1 \omega_2 |M|^2 \quad (7.3.3)$$

where

$$\begin{aligned}
M = & \langle f | \hat{p} \cdot \hat{a}_{\ell_2 m_2}^{\lambda_2}(k_2)^* G(E_i - \hbar\omega_1) \hat{a}_{\ell_1 m_1}^{\lambda_1}(k_1)^* \cdot \hat{p} | i \rangle \\
& + \langle f | \hat{p} \cdot \hat{a}_{\ell_1 m_1}^{\lambda_1}(k_1)^* G(E_i - \hbar\omega_2) \hat{a}_{\ell_2 m_2}^{\lambda_2}(k_2)^* \cdot \hat{p} | i \rangle \\
& + m/2 \langle f | \hat{a}_{\ell_1 m_1}^{\lambda_1}(k_1)^* \cdot \hat{a}_{\ell_2 m_2}^{\lambda_2}(k_2)^* | i \rangle .
\end{aligned} \tag{7.3.4}$$

We are here only interested in the transition from the  $|2s\rangle$  to the  $|1s\rangle$  state which simplifies the angular part of the calculation somewhat. Noting that

$$\nabla [f(r) Y_{00}(\theta, \varphi)] = -df/dr \cdot \hat{Y}_{010}(\theta, \varphi)$$

and expanding  $G$  in spherical harmonics we see that the angular integrals in the Green function part of  $M$  can be performed once we know

$$I_{\ell' m'}^{\ell m \lambda} = \int \hat{Y}_{010}^* \cdot \hat{Y}_{\ell \ell + \lambda m} Y_{\ell' m'} d\Omega . \tag{7.3.5}$$

Now

$$\begin{aligned}
\hat{Y}_{010}^* \cdot \hat{Y}_{\ell \ell + \lambda m} &= \sum_{m_1 m_2} (-1)^{\ell + \lambda - 1 - m} \sqrt{2\ell + 1} Y_{1 m_2}^* Y_{\ell + \lambda m_1} \\
&\times \begin{bmatrix} 1 & 1 & 0 \\ m_1 & -m_2 & 0 \end{bmatrix} \begin{bmatrix} \ell + \lambda & 1 & \ell \\ m_1 & -m_2 & -m \end{bmatrix}
\end{aligned} \tag{7.3.6}$$

so that the problem reduces to integrating the product of three spherical harmonics<sup>29</sup>, with the result that

$$\begin{aligned}
I_{\ell' m'}^{\ell m \lambda} &= (-1)^{\ell + 1 + m} [\ell, \ell + \lambda]^{\frac{1}{2}} / \sqrt{4\pi} \begin{bmatrix} 1 & \ell + \lambda & \ell \\ 0 & 0 & 0 \end{bmatrix} \delta_{\ell, \ell'} \delta_{m, -m'} \\
(7.3.7)
\end{aligned}$$

Hence

$$f_{\ell' m'}^{\ell m 0} = 0, \quad (7.3.8a)$$

$$f_{\ell' m'}^{\ell m+1} = (-1)^m \sqrt{(\ell+1)/4\pi} \delta_{\ell, \ell'} \delta_{m, -m'}, \quad (7.3.8b)$$

$$f_{\ell' m'}^{\ell m-1} = (-1)^m \sqrt{\ell/4\pi} \delta_{\ell, \ell'} \delta_{m, -m'}, \quad (7.3.8c)$$

so that finally

$$\int \tilde{Y}_{010}^* \tilde{a}_{\ell m}^0(k)^* Y_{\ell m'} d\Omega = 0; \quad (7.3.9a)$$

$$\begin{aligned} \int \tilde{Y}_{010}^* \tilde{a}_{\ell m}^{+1}(k)^* Y_{\ell m'} d\Omega &= \delta_{\ell, \ell'} \delta_{m, m'} \sqrt{\ell(\ell+1)/(2\ell+1)4\pi} [g_{\ell+1}^* - g_{\ell-1}^*] \\ &= \delta_{\ell, \ell'} \delta_{m, m'} \sqrt{\ell(\ell+1)/(2\ell+1)4\pi} g_{\ell}^*(kr)/kr \end{aligned} \quad (7.3.9b)$$

where at the final step we have employed a property of spherical Bessel functions and explicitly exhibited the dependence on  $r$  and  $k$ .

Thus

$$\begin{aligned} I_1 &= \langle 1s | \vec{p} \cdot \tilde{a}_{\ell_2 m_2}^1(k_2)^* G(E_{2s} - \hbar\omega_1) \tilde{a}_{\ell_1 m_1}^1(k_1) \cdot \vec{p} | 2s \rangle \\ &= 4\pi\hbar^2/k_1 k_2 (-1)^{\ell+m_1} \ell(\ell+1)(2\ell+1) \delta_{m_1, -m_2} \delta_{\ell, \ell_1} \delta_{\ell, \ell_2} \\ &\quad \times \int R_{1s}'(r_2) j_{\ell}(k_2 r_2) g_{\ell}(r_2, r_1; \nu_1) j_{\ell}(k_1 r_1) R_{2s}'(r_1) r_1 r_2 dr_1 dr_2, \end{aligned} \quad (7.3.10)$$

with all other terms involving the Green function zero.

The angular integrals in the other term in  $M$  (independent of the Green function) can be calculated by noting that

$$\int \tilde{Y}_{\ell\ell+\lambda m}^* \tilde{Y}_{\ell\ell+\lambda' m'} d\Omega = \delta_{\ell\ell'} \delta_{\lambda\lambda'} \delta_{mm'}. \quad (7.3.11)$$

Then

$$\begin{aligned} \langle 1s | \tilde{a}_{\ell_1 m_1}^0(k_1)^* \cdot \tilde{a}_{\ell_2 m_2}^0(k_2)^* | 2s \rangle = \\ (-1)^{\ell_1+m_1+1} (4\pi)^2 \delta_{\ell_1 \ell_2} \delta_{m_1-m_2} \int R_{1s}(r) j_{\ell_1}(k_1 r) j_{\ell_2}(k_2 r) R_{2s}(r) r^2 dr, \end{aligned} \quad (7.3.12a)$$

$$\langle 1s | \tilde{a}_{\ell_1 m_1}^0(k_1)^* \cdot \tilde{a}_{\ell_2 m_2}^{+1}(k_2)^* | 2s \rangle = 0, \quad (7.3.12b)$$

$$\begin{aligned} \langle 1s | \tilde{a}_{\ell_1 m_1}^{+1}(k_1)^* \cdot \tilde{a}_{\ell_2 m_2}^{+1}(k_2)^* | 2s \rangle = (-1)^{\ell_1+m_1} \delta_{\ell_1 \ell_2} \delta_{m_1-m_2} (4\pi)^2 / (2\ell_1+1) \\ \times \int R_{1s}(r) [\ell_1 j_{\ell_1+1}(k_1 r) j_{\ell_2+1}(k_2 r) + (\ell_1+1) j_{\ell_1-1}(k_1 r) j_{\ell_2-1}(k_2 r)] R_{2s}(r) r^2 dr. \end{aligned} \quad (7.3.12c)$$

We must now evaluate the radial integrals. Conservation of energy requires that  $E_{2s} - E_{1s} = \hbar(\omega_1 + \omega_2)$ ; we are thus lead to introduce the dimensionless parameter  $x$ , defined by  $\omega_1 = x(\omega_1 + \omega_2)$  so that

$$\omega_1 = x \frac{3}{8} (\alpha Z)^2 mc^2 / \hbar, \quad \omega_2 = (1-x) \frac{3}{8} (\alpha Z)^2 mc^2 / \hbar,$$

$$k_1 = \omega_1 / c, \quad k_2 = \omega_2 / c$$

$$\text{and } \nu_1 = 2/\sqrt{1+3x}, \quad \nu_2 = 2/\sqrt{4-3x}.$$

The radial functions are given by

$$R_{1s}(r) = 2/a^{3/2} e^{-r/a}, \quad R'_{1s}(r) = -2/a^{5/2} e^{-r/a};$$

$$R_{2s}(r) = 1/a^{3/2} \sqrt{2} (1-r/2a) e^{-r/2a}, \quad R'_{2s}(r) = -1/a^{5/2} \sqrt{2} (1-r/4a) e^{-r/2a}.$$

Thus  $I_1$  can be written as.

$$\begin{aligned}
 I_1 &= m\ell(\ell+1)(2\ell+1) (8/3\alpha Z)^{22\sqrt{2}} 1/a^3 1/x(1-x) (2/a\nu_1)^{2\ell+1} \\
 &\times \sum_{n=0}^{\infty} \frac{n!}{(2\ell+1+n)!(\ell+1+n-\nu_1)} \\
 &\times \int_0^{\infty} e^{-r/a} j_{\ell}(k_2 r) r^{\ell+1} e^{-r/a\nu_1} L_n^{2\ell+1}(2r/a\nu_1) dr \\
 &\times \int_0^{\infty} (1-r/4a) e^{-r/2a} j_{\ell}(k_1 r) r^{\ell+1} e^{-r/a\nu_1} L_n^{2\ell+1}(2r/a\nu_1) dr \quad (7.3.13)
 \end{aligned}$$

All of the integrals involved have been done in Chapter 5. However, in this case we can make things even simpler by eliminating the extra factor of  $r$  in the second integral using the following recursion relation for Laguerre polynomials:

$$\begin{aligned}
 rL_n^{2\ell+1}(2r/a\nu) &= (a\nu/2)[2(\ell+1+n)L_n^{2\ell+1}(2r/a\nu) - \\
 &\quad (n+2\ell+1)L_{n-1}^{2\ell+1}(2r/a\nu) - (n+1)L_{n+1}^{2\ell+1}(2r/a\nu)] \quad (7.3.14)
 \end{aligned}$$

Now all the integrals can be written in basically the same form, the general expression having been given in (5.3.8). Defining

$$f_n^{\ell}(\theta) = \sum_{i=0}^{\ell} \frac{(n+i)!}{(n+\ell+1+i)!} \left[ \begin{matrix} \ell \\ i \end{matrix} \right] (-1)^i \sin([n+2i+1]\theta) \quad (7.3.15)$$

we find

$$\begin{aligned}
I_1 = & A_\ell \sum_{n=0}^{\infty} \frac{(2\ell+1+n)!}{n!(\ell+1+n-\nu_1)} (X_1 X_2)^n f_n^\ell(\theta_1) \\
& \times \left[ [1-\nu_1(\ell+1+n)/4] f_n^\ell(\theta_2) + \nu_1 n/(8X_2) f_{n-1}^\ell(\theta_2) + \nu_1(n+2\ell+2)X_2/8 f_{n+1}^\ell(\theta_2) \right],
\end{aligned}
\tag{7.3.16}$$

where

$$\begin{aligned}
X_1 &= ([16(2-\sqrt{1+3x})^2 + 9(1-x)^2(\alpha Z)^2]/[16(2+\sqrt{1+3x})^2 + 9(1-x)^2(\alpha Z)^2])^{\frac{1}{2}}, \\
X_2 &= -([16(1-\sqrt{1+3x})^2 + 9x^2(\alpha Z)^2]/[16(1+\sqrt{1+3x})^2 + 9x^2(\alpha Z)^2])^{\frac{1}{2}}, \\
\tan\theta_1 &= 8\sqrt{1+3x} (\alpha Z)/[16+3(1-x)(\alpha Z)^2], \\
\tan\theta_2 &= -8\sqrt{1+3x} (\alpha Z)/[16-3x(\alpha Z)^2],
\end{aligned}
\tag{7.3.17}$$

and

$$\begin{aligned}
A^\ell = & \ell(\ell+1)(2\ell+1) \sqrt{2}/2^{2\ell+1} (8/3(\alpha Z))^2 1/x(1-x) (a\nu_1)^{2\ell+3} \\
& \times (1/c_1 c_2)^\ell 1/k_1 k_2 X_1 X_2,
\end{aligned}
\tag{7.3.18}$$

with

$$\begin{aligned}
c_1 &= 24(1-x)\sqrt{1+3x} (\alpha Z)/[16(2-\sqrt{1+3x})^2 + 9(1-x)^2(\alpha Z)^2], \\
c_2 &= 24x \sqrt{1+3x} (\alpha Z)/[16(1+\sqrt{1+3x})^2 + 9x^2(\alpha Z)^2].
\end{aligned}
\tag{7.3.19}$$

Three possible singularities appear at first sight in  $I_1$ . At  $x=0$  and  $x=1$  we might expect the integral to diverge; nonetheless this does not actually happen. For example,

$$16(1-\sqrt{1+3x})^2+9x^2(\alpha Z)^2 = 9x^2[(\alpha Z)^2+ 16/(1+\sqrt{1+3x})] \quad (7.3.20)$$

has a factor of  $x$  which cancels one  $x$  in the denominator. When  $\ell=1$  and  $\bar{n}=0$ ,  $(\ell+1+n-\nu)=(2-2/\sqrt{1+3x})$  becomes zero at  $x=0$ , but this singularity is cancelled by the terms in  $X_2$ . Finally, the dependence on  $(\alpha Z)$  to zeroth order (or lower) due to the terms in the denominator of  $A^\ell$  is also illusory. The integral is actually of order  $(\alpha Z)^{2\ell-2}$ . That this is so is due to an amusing property of the finite sum,  $f_n^\ell(\theta)$ . Expanding  $\sin\theta$  as a power series in  $\theta$  we find that

$$\lim_{\theta \rightarrow 0} f_n^\ell(\theta) \approx \theta^{2\ell+1} \quad (7.3.21)$$

independently of  $n$ , since the finite sums for the lower order terms are identically equal to zero.

The integrals in (7.3.12c) have been given by Morse and Feshbach. They can also be calculated by an addition theorem for the spherical Bessel functions (see Lebedev<sup>39</sup>). The integrals in each particular case are tedious and will not be presented here; none the less it should be immediately apparent that the term in (7.3.4) independent of the Green function is of relative order  $(\alpha Z)^2$  compared with the other terms.

I have performed the above integral for the E1E1 transition ( $\ell=1, \lambda=0$ ) in hydrogenic ions. The computations agree well with previous reports; the  $Z=0$  case exactly reproduces the long wavelength approximation calculation made by Klarsfeld<sup>50</sup>. The fully relativistic calculations by Goldman and Drake<sup>3</sup> include terms in  $(\alpha Z)$  due both to retardation (which I have included) and to relativistic effects (which I have excluded). In Table 1 I present the values for the spectral distribution at  $\alpha Z=0$

obtained in the present calculation, together with Klarsfeld's<sup>50</sup> results. In Table 2 I compare the spectral density values obtained here for  $Z=1,20$  with those obtained by Goldman and Drake.<sup>3</sup> As is apparent the agreement is good, though fully relativistic calculations using the radial integrals derived in Chapter 5 are obviously required to reach complete agreement. Nonetheless, I hope to have shown that the general methods described in this dissertation are applicable to specific calculations, though their applicability goes far beyond two photon transitions.



TABLE 1 :  
SPECTRAL DISTRIBUTION IN THE LONG WAVELENGTH APPROXIMATION

$x = \omega_1 / \omega_2 + \omega_1$	Present work	Klarsfeld <sup>50</sup>
0.00	0.00	0.00
0.05	1.7228	1.723
0.10	2.7773	2.777
0.15	3.4713	3.471
0.20	3.9485	3.949
0.25	4.2845	4.284
0.30	4.5223	4.522
0.35	4.6878	4.688
0.40	4.7968	4.797
0.45	4.8588	4.859
0.50	4.8790	4.879

TABLE 2 :  
SPECTRAL DISTRIBUTION FOR Z=1 & Z=20

	$x=\omega_1/\omega_1+\omega_1$	Present work	Goldman & Drake <sup>3</sup>
Z=1	.0625	2.0326	2.0324
	.1250	3.1581	3.1579
	.1875	3.8446	3.8445
	.2500	4.2844	4.2844
	.3125	4.5696	4.5696
	.3750	4.7486	4.7486
	.4375	4.8473	4.8473
	.5000	4.8789	4.8789
Z=20	.0625	2.0217	1.9447
	.1250	3.1428	3.0852
	.1875	3.8280	3.7863
	.2500	4.2679	4.2383
	.3125	4.5537	4.5331
	.3750	4.7334	4.7189
	.4375	4.8326	4.8217
	.5000	4.8644	4.8546

## APPENDIX A.1 : SPECIAL FUNCTIONS

*Hypergeometric Functions*

$$(\alpha)_n = \Gamma(\alpha+n)/\Gamma(\alpha)$$

$${}_1F_1(\alpha; \beta; x) = \sum \frac{(\alpha)_n}{(\beta)_n} \frac{x^n}{n!}$$

$${}_2F_1(\alpha, \beta; \gamma; x) = \sum \frac{(\alpha)_n (\beta)_n}{(\gamma)_n} \frac{x^n}{n!}$$

$${}_pF_q(\alpha_1, \dots; \beta_1, \dots; x) = \sum \frac{(\alpha_1)_n \dots (\alpha_p)_n}{(\beta_1)_n \dots (\beta_q)_n} \frac{x^n}{n!}$$

*Vandermonde's Theorem*

$${}_2F_1(-n, b; c; 1) = (c-b)_n / (c)_n$$

*Laguerre Polynomials*

$$L_n^\alpha(x) = \frac{\Gamma(\alpha+1+n)}{\Gamma(\alpha+1) n!} {}_1F_1(-n; \alpha+1; x)$$

$$(n+1)L_{n+1}^\alpha(x) + (x-\alpha-2n-1)L_n^\alpha(x) + (n+\alpha)L_{n-1}^\alpha(x) = 0$$

*Whittaker Functions* (see Buchholz<sup>40</sup>)

$$\begin{aligned} M_{\nu, \lambda}(x) &= x^{\lambda+\frac{1}{2}} e^{-x/2} {}_1F_1(\lambda+1/2-\nu; 2\lambda+1; x) \\ &= x^{\lambda+\frac{1}{2}} e^{+x/2} {}_1F_1(\lambda+1/2+\nu; 2\lambda+1; -x) \end{aligned}$$

$$W_{\nu,\lambda}(x) = \frac{\Gamma(-2\lambda)}{\Gamma(1/2-\lambda-\nu)} M_{\nu,\lambda}(x) + \frac{\Gamma(2\lambda)}{\Gamma(1/2+\lambda-\nu)} M_{\nu,-\lambda}(x)$$

$$(1+2\lambda)\frac{d}{dx} M_{\nu,\lambda}(x) = [(1+2\lambda)^2/2x - \nu] M_{\nu,\lambda}(x) - [\nu^2 - (1/2+\lambda/2)^2]/(2+2\lambda)(1+2\lambda) M_{\nu,\lambda+1}(x)$$

$$(1-2\lambda)\frac{d}{dx} M_{\nu,\lambda}(x) = [(1-2\lambda)^2/2x - \nu] M_{\nu,\lambda}(x) - (2\lambda+1)(2\lambda) M_{\nu,\lambda-1}(x)$$

$$(1+2\lambda)\frac{d}{dx} W_{\nu,\lambda}(x) = [(1+2\lambda)^2/2x - \nu] W_{\nu,\lambda}(x) + [\nu - 1/2 - \lambda] W_{\nu,\lambda+1}(x)$$

$$(1-2\lambda)\frac{d}{dx} W_{\nu,\lambda}(x) = [(1-2\lambda)^2/2x - \nu] W_{\nu,\lambda}(x) + [\nu - 1/2 + \lambda] W_{\nu,\lambda-1}(x)$$

$\int$   
Bessel functions.

$$J_{\nu}(z) = \sum_{k=0}^{\infty} \frac{(-1)^k (z/2)^{\nu+2k}}{\Gamma(k+1)\Gamma(k+\nu+1)}$$

$$I_{\nu}(z) = \sum_{k=0}^{\infty} \frac{(z/2)^{\nu+2k}}{\Gamma(k+1)\Gamma(k+\nu+1)}$$

$$j_{\ell}(z) = \sqrt{2/\pi z} J_{\ell+1/2}(z)$$

Dirac Matrices

$$\alpha = \begin{bmatrix} 0 & \partial \\ \partial & 0 \end{bmatrix}, \quad \beta = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \partial = \left[ \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \right]$$

# APPENDIX B.1 : CALCULATION OF SOME INTEGRALS REQUIRED FOR THE NORMALIZATION OF WAVEFUNCTIONS

Several methods of obtaining these integrals are known. However, the following are simple proofs requiring only a knowledge of Vandermonde's theorem (Appendix A.1).

(i)

$$\begin{aligned}
 & \int_0^\infty e^{-x} x^\alpha {}_1F_1(-n; \alpha; x)^2 dx \\
 &= \sum_{i=0}^n \sum_{j=0}^n \left[ \begin{matrix} n \\ i \end{matrix} \right] \left[ \begin{matrix} n \\ j \end{matrix} \right] (-1)^{i+j} \frac{\Gamma(\alpha)^2}{\Gamma(\alpha+i)\Gamma(\alpha+j)} \int_0^\infty e^{-x} x^{\alpha+i+j} dx \\
 &= \sum_{i=0}^n \left[ \begin{matrix} n \\ i \end{matrix} \right] (-1)^i \frac{\Gamma(\alpha)\Gamma(\alpha+i+1)}{\Gamma(\alpha+i)} {}_2F_1(-n, \alpha+i+1; \alpha+1; 1) \\
 &= \sum_{i=0}^n \left[ \begin{matrix} n \\ i \end{matrix} \right] (-1)^i \frac{\Gamma(\alpha)\Gamma(\alpha+i+1)}{\Gamma(\alpha+i)} \frac{(-i-1)_n}{(\alpha)_n} \\
 &= \frac{\Gamma(\alpha)^2 (\alpha+2n)}{\Gamma(\alpha+n)} n! \quad (B.1.1)
 \end{aligned}$$

Hence

$$\int_0^\infty e^{-x} x^\alpha [L_n^{\alpha-1}(x)]^2 dx = (\alpha+2n)\Gamma(\alpha+n)/n! \quad (B.1.2)$$

(ii)

$$\int_0^\infty e^{-x} x^{\alpha+1} {}_1F_1(-n; \alpha; x) {}_1F_1(-n+1; \alpha+2; x) dx = -2 \frac{\Gamma(\alpha)\Gamma(\alpha+2)}{\Gamma(\alpha+n)} n! \quad (B.1.3)$$

$$\int_0^{\infty} e^{-x} x^{\alpha+1} L_n^{\alpha-1}(x) L_{n-1}^{\alpha+1}(x) dx = -2 \Gamma(\alpha+n+1)/n! . \quad (\text{B.1.4})$$

(iii)

$$\int_0^{\infty} e^{-x} x^{\alpha} {}_1F_1(-n; \alpha+1; x)^2 dx = \frac{\Gamma(\alpha+1)^2}{\Gamma(\alpha+1+n)} n! , \quad (\text{B.1.5})$$

$$\int_0^{\infty} e^{-x} x^{\alpha} [L_n^{\alpha}(x)]^2 dx = \Gamma(\alpha+n+1)/n! . \quad (\text{B.1.6})$$

The last two Laplace transforms were derived in exactly the same manner as the first, by expanding the confluent hypergeometric functions, integrating, and using Vandermonde's theorem once.

## APPENDIX B.2 : A SIMPLIFIED FORM OF $F_1$ WHEN TWO PARAMETERS ARE INTEGERS.

In this appendix we show that the Appell hypergeometric function of two variables of the first kind reduces to a finite sum of ordinary hypergeometric functions when the second two parameters are integers. We begin by noting the following two integral representations of hypergeometric functions<sup>44</sup>:

$$F_1(\alpha; \beta, \beta'; \gamma, x, y) = \frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\gamma-\alpha)} \int_0^1 u^{\alpha-1} (1-u)^{\gamma-\alpha-1} (1-ux)^{-\beta} (1-uy)^{-\beta'} du, \quad (B.2.1)$$

for  $\Re(\alpha) > 0$ ,  $\Re(\gamma-\alpha) > 0$ ;

$${}_2F_1(\alpha, \beta; \gamma; z) = \frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\gamma-\alpha)} \int_0^1 u^{\alpha-1} (1-u)^{\gamma-\alpha-1} (1-uz)^{-\beta} du, \quad (B.2.2)$$

for  $\Re(\gamma) > \Re(\alpha) > 0$ .

Let  $\beta = m$ ,  $\beta' = m'$  be integers. Standard reduction to partial fractions shows that

$$\begin{aligned} (1-ux)^{-m} (1-uy)^{-m'} &= \\ &\left[ (-1)^{m'} x^{m'} y^m (y-x)^{-m-m'} \sum_{i=1}^m \frac{(m+m'-i-1)!}{(m-i)!(m'-1)!} \left[ \frac{y-x}{y} \right]^i (1-ux)^{-i} \right. \\ &\quad \left. + (-1)^m x^{m'} y^m (x-y)^{-m-m'} \sum_{i=1}^{m'} \frac{(m+m'-i-1)!}{(m'-i)!(m-1)!} \left[ \frac{x-y}{y} \right]^i (1-uy)^{-i} \right] \quad (B.2.3) \end{aligned}$$

and introducing this into the integral representation (B.2.1) gives immediately

$$\begin{aligned}
 F_1(\alpha; m, m'; \gamma; x, y) &= (-1)^m x^{m'} y^m (x-y)^{-m-m'} \\
 &\times \left[ \sum_{i=1}^m \frac{(m+m'-i-1)!}{(m-i)!(m'-1)!} \left[ \frac{x-y}{y} \right]^i {}_2F_1(\alpha, i; \gamma; x) \right. \\
 &\quad \left. + \sum_{i=1}^{m'} \frac{(m+m'-i-1)!}{(m'-i)!(m-1)!} \left[ \frac{y-x}{x} \right]^i {}_2F_1(\alpha, i; \gamma; y) \right], \quad (B.2.4)
 \end{aligned}$$

which is the required result.



# APPENDIX B.3: THE LAPLACE TRANSFORM OF THE SPHERICAL BESSEL FUNCTION

In this appendix I briefly sketch the calculation of the following integral:

$$I_n(a, b, c) = \int_0^\infty e^{-a\sigma} \sigma^b j_n(c\sigma) d\sigma, \quad \Re(a) > 0, \Re(b) > -1. \quad (\text{B.3.1})$$

The trick we use to derive the formula given in Chapter 6 is to express the spherical Bessel function as an integral over a Legendre polynomial thus:

$$j_n(c\sigma) = 1/2 (-i)^n \int_{-1}^{+1} e^{ic\sigma\tau} P_n(\tau) d\tau \quad (\text{B.3.2})$$

where  $P_n(\tau) = 1/(2^n n!) d^n/d\tau^n (\tau^2 - 1)^n$ . Changing the order of integration gives

$$\begin{aligned} I_n(a, b, c) &= 1/2 (-i)^n \int_{-1}^{+1} P_n(\tau) \int_0^\infty e^{-(a-ic\tau)\sigma} \sigma^b d\sigma d\tau \\ &= 1/2 (-i)^n \int_{-1}^{+1} P_n(\tau) \frac{\Gamma(b+1)}{(a-ic\tau)^{b+1}} d\tau. \end{aligned} \quad (\text{B.3.3})$$

Noting the definition of  $P_n$  and integrating by parts leads finally to

$$\begin{aligned} I_n(a, b, c) &= 1/2 (i)^{b+1-n} c^{-n-1} \frac{\Gamma(b+1+n)\Gamma(b-n)}{2^n \Gamma(b+1)} \\ &\times \left[ (ia-c)^{n-b} {}_2F_1(-n, b-n; b+1; \frac{ia+c}{ia-c}) - (ia+c)^{n-b} {}_2F_1(-n, b-n; b+1; \frac{ia-c}{ia+c}) \right] \end{aligned} \quad (\text{B.3.4})$$

$$= (1/2c)^{n+1} (a^2+c^2)^{n-b} (-i)^{b+1-n} \frac{\Gamma(b+1+n)\Gamma(b-n)}{\Gamma(b+1)} \\ \times \left[ (ia-c)^{b-n} {}_2F_1(-n, b-n; b+1; \frac{ia-c}{ia+c}) - (ia+c)^{b-n} {}_2F_1(-n, b-n; b+1; \frac{ia+c}{ia-c}) \right] \quad (B.3.5)$$

for  $b$  non-integral or for  $b$  an integer greater than  $n$ . The solution is obviously real as a brief inspection of the complex conjugate will show. It can be quite readily shown that the following explicitly real expression is equivalent to (B.3.5) with  $\tan \theta = c/a$ :

$$I_n(a, b, c) = \frac{\Gamma(b+1+n)\Gamma(b-n)}{2^n \Gamma(b+1)} c^{-n-1} (a^2+c^2)^{\frac{1}{2}(n-b)} \\ \times \sum_{m=0}^n \left[ \begin{matrix} n \\ m \end{matrix} \right] \frac{\Gamma(b-n+m)\Gamma(b+1)}{\Gamma(b-n)\Gamma(b+1+m)} (-1)^m \sin([b-n+2m]\theta) \quad (B.3.6)$$

Using Vandermonde's Theorem for the summation of finite hypergeometric functions at the appropriate point it can be shown that (B.3.6) implies that

$$I_n(a, b, 0) = \frac{\Gamma(b+1)}{a^{b+1}} \delta_{n,0}, \quad (B.3.7)$$

which is immediately clear from (B.3.1).

It is possible to express (B.3.4) in a somewhat different form:

$${}_2F_1(-n, b-n; b+1; \frac{ia+c}{ia-c}) = \sum_{m=0}^n \left[ \begin{matrix} n \\ m \end{matrix} \right] (-1)^m \frac{\Gamma(b-n+m)\Gamma(b+1)}{\Gamma(b-n)\Gamma(b+1+m)} \left[ \frac{ia+c}{ia-c} \right]^m \\ = \sum_{m=0}^n \left[ \begin{matrix} n \\ m \end{matrix} \right] (-1)^m \frac{\Gamma(b-n+m)\Gamma(b+1)}{\Gamma(b-n)\Gamma(b+1+m)} \sum_{k=0}^m \left[ \begin{matrix} m \\ k \end{matrix} \right] \left[ \frac{2c}{ia-c} \right]^k \\ = \sum_{k=0}^n \left[ \begin{matrix} n \\ k \end{matrix} \right] (-1)^k \frac{\Gamma(b+1)\Gamma(b-n+k)}{\Gamma(b+1+k)\Gamma(b-n)} \left[ \frac{2c}{ia-c} \right]^k {}_2F_1(-n+k, b-n+k; b+1+k; 1)$$

which can be simplified by using Vandemonde's theorem. Hence

$${}_2F_1(-n, b-n; b+1; \frac{ia+c}{ia-c}) = \frac{\Gamma(b+1)}{\Gamma(b+1+n)} \frac{(2n)!}{n!} {}_2F_1(-n, b-n; -2n; \frac{2c}{ia-c}) \quad (B.3.8)$$

It is now possible to rewrite (B.3.4) :

$$I_n(a, b, c) = \frac{\Gamma(b-n)(2n)!}{2^{n+1}n!} (i)^{b+1-n} c^{-n-1} \left[ (ia-c)^{n-b} {}_2F_1(-n, b-n; -2n; \frac{2c}{ia-c}) - (ia+c)^{n-b} {}_2F_1(-n, b-n; -2n; \frac{2c}{ia+c}) \right] \quad (B.3.9)$$

$$= - \frac{\Gamma(b-n)(2n)!}{2^n n!} c^{-n-1} (a^2+c^2)^{\frac{1}{2}(n-b)} \sum_{m=0}^n \begin{bmatrix} n \\ m \end{bmatrix} \frac{(2n-m)!\Gamma(b-n+m)}{(2n)!\Gamma(b-n)} (2c/\sqrt{a^2+c^2})^m \sin([n-b-m]\theta + m\pi/2) \quad (B.3.10)$$

An alternative, and perhaps more familiar form of  $I_n(a, b, c)$  can be found when  $b$  is an integer greater than  $n$ ,  $b = n+1+k$ . Then

$$\begin{aligned} I_n(a, n+1+k, c) &= \sqrt{\pi/2c} \int_0^\infty \sigma^{n+\frac{1}{2}+k} e^{-a\sigma} J_{n+\frac{1}{2}}(c\sigma) d\sigma \\ &= \sqrt{\pi/2c} (-1)^k \frac{d^k}{da^k} \int_0^\infty \sigma^{n+\frac{1}{2}} e^{-a\sigma} J_{n+\frac{1}{2}}(c\sigma) d\sigma \\ &= \sqrt{\pi/2c} (-1)^k \frac{d^k}{da^k} n!/\sqrt{\pi} (2c)^{n+\frac{1}{2}} (a^2+c^2)^{-n-1} \\ &= k!n! (2c)^n (a^2+c^2)^{-n-1-k/2} C_k^{n+1} (a/(a^2+c^2)^{\frac{1}{2}}) \quad (B.3.11) \end{aligned}$$

where  $C_k^n$  is a Gegenbauer polynomial of degree  $k$ . Notice that in this solution we have  $k$  terms, whereas in the previous solution we had  $n$  terms.

Depending on which of  $n$  or  $k$  is integral will determine our choice of

solutions.

We can use the preceding Laplace transforms of the spherical Bessel function to derive a slightly more general result involving Laguerre polynomials. Since the proof simply involves expanding the Laguerre polynomial in powers and using the previous results for each term I will be satisfied to present the final result.

$$I_{n,k}^{\alpha}(a,b,c) \equiv \int_0^{\infty} e^{-a\sigma} \sigma^b L_k^{\alpha}(\sigma) j_n(c\sigma) d\sigma \quad (\text{B.3.12})$$

$$= \frac{\Gamma(\alpha+1+k)}{n! k!} (1/2c)^{n+1} i^{b+1-n} \sum_{m=0}^n \left[ \begin{matrix} n \\ m \end{matrix} \right] \frac{(2n-m)! \Gamma(b-n+m)}{\Gamma(\alpha+1)} (2c)^m \\ \times \left[ (-1)^m (ia-c)^{n-b-m} {}_2F_1(-k, b+m-n; \alpha+1; \frac{i}{ia-c}) \right. \\ \left. - (ia+c)^{n-b-m} {}_2F_1(-k, b+m-n; \alpha+1; \frac{i}{ia+c}) \right] \quad (\text{B.3.13})$$

$$= -2 \frac{\Gamma(\alpha+1+k)}{n! k!} (1/2c)^{n+1} (a^2+c^2)^{\frac{1}{2}}(n-b) \\ \times \sum_{m=0}^n \left[ \begin{matrix} n \\ m \end{matrix} \right] \frac{(2n-m)! \Gamma(b-n+m)}{\Gamma(\alpha+1)} \left[ \frac{2c}{\sqrt{a^2+c^2}} \right]^m \sum_{i=0}^k \left[ \begin{matrix} k \\ i \end{matrix} \right] \frac{\Gamma(b+m-n+i) \Gamma(\alpha+1)}{\Gamma(b+m-n) \Gamma(\alpha+1+i)} \\ \times (1/\sqrt{a^2+c^2})^i \sin([n-b-m-i]\theta + m\pi/2) \quad (\text{B.3.14})$$

APPENDIX B.4 : ON THE FUNCTION  ${}_2F_1(M+N+1,1;N+1;X)$ 

It is known that<sup>39</sup>

$${}_2F_1(\alpha-1, \beta+1; \gamma; x) - {}_2F_1(\alpha, \beta; \gamma; x) = x(\alpha-\beta-1)/\gamma {}_2F_1(\alpha, \beta+1; \gamma+1; x) \quad (\text{B.4.1})$$

from which it follows (by induction) that

$${}_2F_1(m+n+1, 1; n+1; x) = \frac{n!}{(m+n)!} \left[ -\sum_{k=1}^n \frac{(m+n-k)!}{(n-k)!} x^{-k} + m! x^{-n} (1-x)^{-m-1} \right] \quad (\text{B.4.2})$$

The last term can be expanded by the method of partial fractions,

$$x^{-n} (1-x)^{-m-1} = (-1)^{m+1} \left[ \sum_{k=1}^n \frac{(m+n-k)!}{(n-k)! m!} x^{-k} + \sum_{k=0}^m \frac{(n-1+k)!}{(n-1)! k!} (1-x)^{k-m-1} \right], \quad (\text{B.4.3})$$

and this leads to the required result:

$${}_2F_1(m+n+1, 1; n+1; x) = \frac{nm!}{(n+m)!} \sum_{k=0}^m \frac{(n-1-k)!}{k!} (1-x)^{k-m-1} \quad (\text{B.4.4})$$

## APPENDIX B.5 : ON A SUM RELATED TO THE LOGARITHM

We wish to calculate

$$f_{m,n}(x) = \sum_{k=0}^{\infty} \frac{(m+n+k)!}{(n+k)! (k+1)} x^{k+1} \quad (\text{B.5.1})$$

where  $m$  and  $n$  are integers. We proceed as follows.

$$\begin{aligned} f_{m,n}(x) &= \sum_{k=0}^{\infty} \frac{(m+n+k)!}{(n+k)!} \int_0^x t^k dt \\ &= \int_0^x \sum_{k=0}^{\infty} \frac{(m+n+k)!}{(n+k)!} t^k dt \\ &= \frac{(m+n)!}{n!} \int_0^x {}_2F_1(m+n+1, 1; n+1; t) dt \quad (\text{B.5.2}) \end{aligned}$$

We have calculated the hypergeometric function in a Appendix B.4. Thus

$$\begin{aligned} f_{m,n}(x) &= \frac{m!}{(n-1)!} \int_0^x \sum_{k=0}^m \frac{(n-1+k)!}{k!} (1-t)^{k-m-1} dt \\ &= \frac{m!}{(n-1)!} \sum_{k=0}^{m-1} \frac{(n-1+k)!}{k! (m-k)} [(1-x)^{k-m} - 1] - \frac{(n+m-1)!}{(n-1)!} \log(1-x), \quad (\text{B.5.3}) \end{aligned}$$

which is the result we desire.

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## VITA AUCTORIS

NAME: Robin Andrew Swainson

BORN: 11th April 1958, Spondon, Derby, England.

EDUCATED:

- \* New College, Oxford, England, 1977-1980, (B.A. in Mathematics)
- \* University of York, England, 1980-1982, (M.Sc. in Mathematics)
- \* University of Windsor, Canada, 1982-1988, (expecting to graduate with a Ph.D. in Physics, Spring 1988).